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7-Bromo-3-ethyl-9-phenyl-2-tosylpyrrolo[3,4-*b*]quinoline

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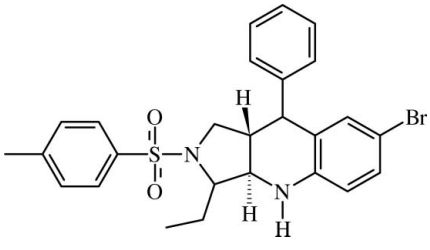
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.094; data-to-parameter ratio = 48.6.

In the title compound, $C_{26}H_{27}BrN_2O_2S$, the pyrrolidine ring adopts a twist conformation, while the tetrahydropyridine ring is in a half-chair conformation. The two rings are *trans*-fused. The dihedral angle between the phenyl ring and the sulfonyl-bound benzene ring is 22.83 (7)°. N—H···O hydrogen bonds link the molecules into a chain along the *b* axis, and the chains are cross-linked into a three-dimensional network by a C—H···π interaction and a weak π-π interaction between the sulfonyl-bound benzene rings; the centroid–centroid distance is 3.6957 (8) Å.

Related literature

The crystal structure of the title compound is similar to that of its chloro analogue (Sudha *et al.*, 2007). For ring puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Duax *et al.* (1976).



Experimental

Crystal data

$C_{26}H_{27}BrN_2O_2S$
M_r = 511.47
Monoclinic, $P2_1/c$
a = 9.6293 (2) Å
b = 13.4574 (3) Å
c = 20.2179 (4) Å
β = 116.930 (1)°
V = 2335.84 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.88 mm^{-1}
T = 100.0 (1) K
0.58 × 0.52 × 0.34 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.323, T_{max} = 0.529
58171 measured reflections
14302 independent reflections
9599 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 1.01
14302 reflections
294 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1N2···O1^{i}	0.83 (2)	2.33 (2)	3.1381 (14)	162 (2)
C25—H25A···O2	0.97	2.49	3.1312 (15)	123
C3—H3···$Cg1^{ii}$	0.98	2.83	3.7921 (12)	168

Symmetry codes: (i) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, -y+1, -z$. $Cg1$ is the centroid of the C4–C9 benzene ring.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); 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: IS2257).

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7-Bromo-3-ethyl-9-phenyl-2-tosylpyrrolo[3,4-*b*]quinoline

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

S1. Comment

Previously, we have reported the crystal structure of 7-chloro-2-ethyl-5-phenyl-3-tosyl-pyrrolo[3,4-*b*]quinoline (Sudha *et al.*, 2007). Now we report here the crystal structure of the bromo analogue, the title compound.

Bond lengths and angles are comparable with those in the chloro analogue (Sudha *et al.*, 2007). A superposition of the non-H atoms (except halides) of the title molecule and its chloro analogue (Fig. 2) using *XP* in *SHELXTL* (Sheldrick, 1998), gave an r.m.s. deviation of 0.868 Å. In both compounds, the pyrrolidine ring is *trans*-fused to the tetrahydropyridine ring.

The pyrrolidine ring has a twist conformation; the asymmetry parameters ΔC_2[C2—C10] (Duax *et al.*, 1976) and the puckering parameters q_2 and φ (Cremer & Pople, 1975) are 0.5 (1)°, 0.481 (1) Å and 270.5 (1)°, respectively. The tosyl group is attached to the pyrrolidine ring in a biaxial position. The tetrahydropyridine ring adopts a half-chair conformation, with Q, θ, φ and ΔC_2[C4—C9] values of 0.461 (1) Å, 44.6 (2)°, 269.1 (2)° and 2.4 (2)°, respectively. The phenyl group is attached to the tetrahydropyridine ring in a biaxial position. The C19—C24 phenyl ring forms dihedral angles of 72.42 (3) and 22.83 (7)°, respectively, with the C4—C9 and C12—C17 benzene rings.

As observed in the isomorphous chloro analogue, the screw-related molecules are linked into a chain along the *b* axis through N—H···O hydrogen bonds and the chains are cross-linked into a three-dimensional framework (Fig. 3) by C—H···π interactions (Table 2) and π-π interactions between the C12—C17 benzene rings of molecules at (*x*, *y*, *z*) and (2 - *x*, 1 - *y*, 1 - *z*) [the centroid-centroid distance is 3.6957 (8) Å].

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 in 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. The highest residual density peak and the deepest hole are located 0.65 and 0.58 Å, respectively, from atom Br1.

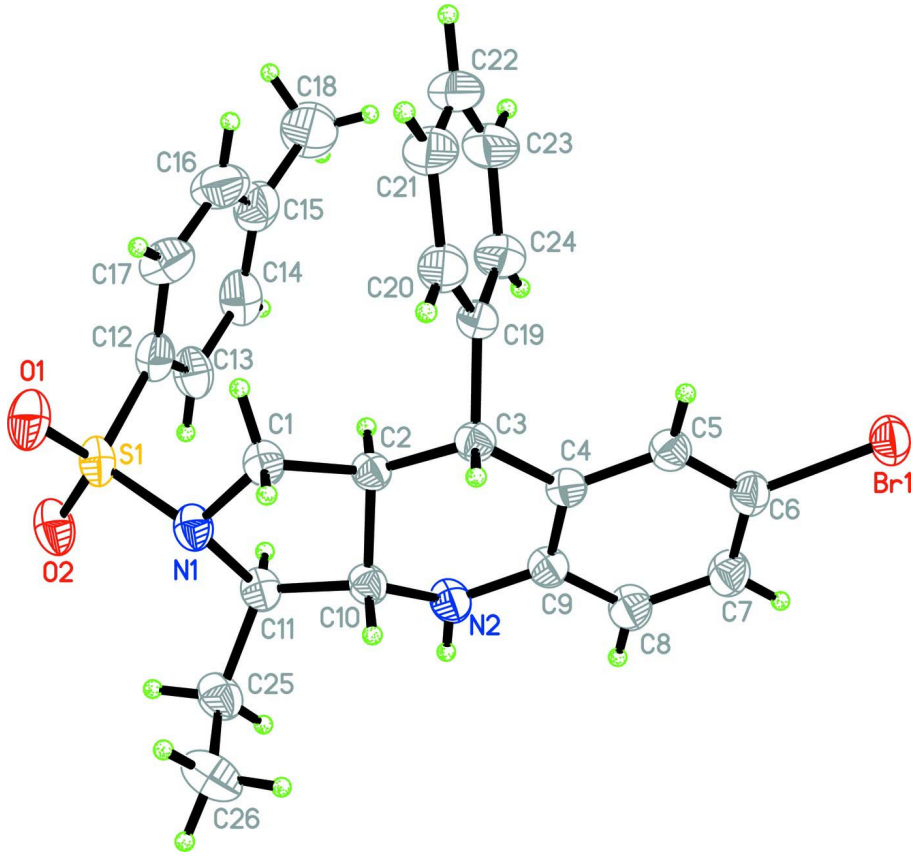

Figure 1

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

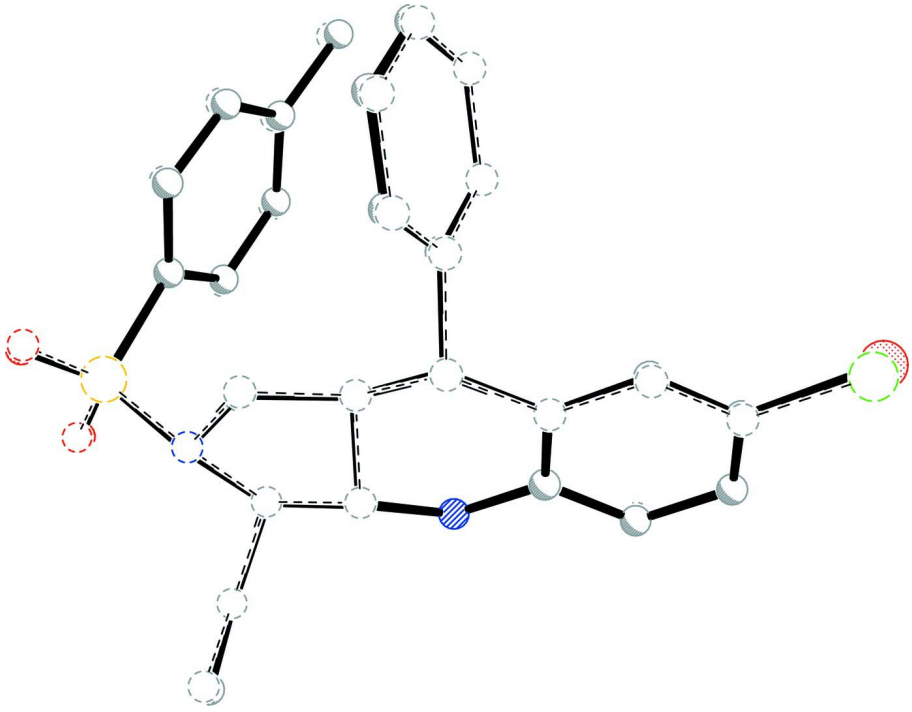

Figure 2

Fit of the title molecule (solid lines) with its chloro analogue (Dashed lines). H atoms have been omitted for clarity.

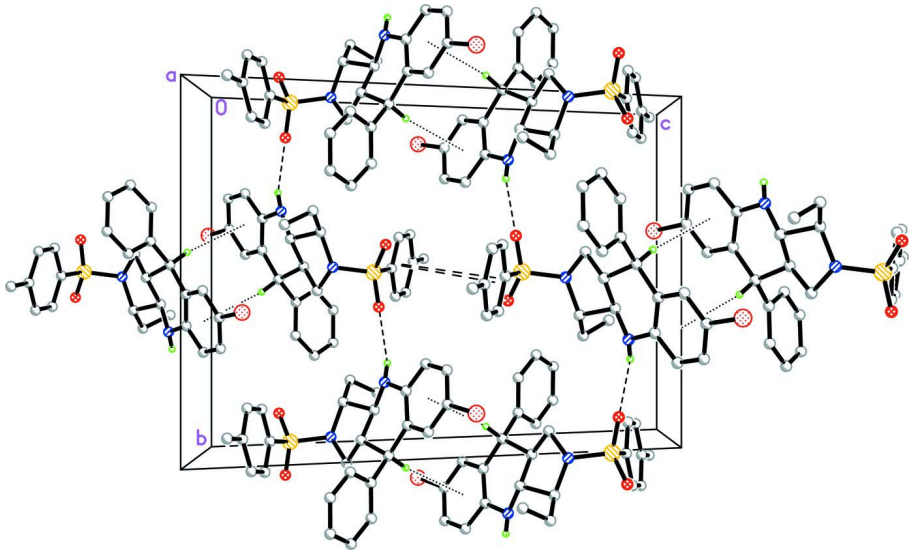

Figure 3

Part of the three-dimensional network in the title compound. Dashed and dotted lines indicate N—H···O and C—H···π interactions, respectively. The π-π interaction is shown by a dashed open line. For the sake of clarity, H atoms not involved in the interactions have been omitted.

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Crystal data

$C_{26}H_{27}BrN_2O_2S$
$M_r = 511.47$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.6293$ (2) Å
$b = 13.4574$ (3) Å
$c = 20.2179$ (4) Å
$\beta = 116.930$ (1)°
$V = 2335.84$ (9) Å^3
$Z = 4$
$F(000) = 1056$
$D_x = 1.454$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5745 reflections
$\theta = 2.4$–$38.4°$
$\mu = 1.88$ mm^{-1}
$T = 100$ K
Block, colourless
0.58 × 0.52 × 0.34 mm

Data collection

Bruker SMART 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)
$T_{min} = 0.323$, $T_{max} = 0.529$
58171 measured reflections
14302 independent reflections
9599 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 40.0°$, $\theta_{min} = 2.3°$
$h = -16\rightarrow17$
$k = -24\rightarrow23$
$l = -36\rightarrow36$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.094$
$S = 1.01$
14302 reflections
294 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
$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 0.5198P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.13$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ 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}
Br1	0.009166 (12)	0.383484 (9)	−0.061858 (7)	0.01903 (3)
S1	1.10805 (3)	0.50065 (2)	0.342333 (16)	0.01644 (5)

O1	1.16380 (10)	0.60150 (7)	0.35422 (6)	0.02221 (18)
O2	1.21739 (10)	0.42008 (7)	0.36992 (5)	0.02180 (17)
N1	1.00957 (10)	0.48551 (7)	0.25246 (6)	0.01539 (16)
N2	0.70188 (11)	0.31729 (7)	0.13123 (6)	0.01682 (17)
H1N2	0.738 (2)	0.2632 (16)	0.1260 (10)	0.024 (4)*
C1	0.87389 (12)	0.55496 (8)	0.21501 (6)	0.01499 (18)
H1A	0.8835	0.5940	0.1770	0.018*
H1B	0.8642	0.5993	0.2505	0.018*
C2	0.73638 (11)	0.48360 (8)	0.18133 (6)	0.01310 (16)
H2	0.7174	0.4574	0.2217	0.016*
C3	0.58180 (11)	0.52210 (8)	0.12093 (6)	0.01333 (16)
H3	0.6032	0.5603	0.0853	0.016*
C4	0.48065 (12)	0.43277 (8)	0.08039 (6)	0.01331 (16)
C5	0.32017 (12)	0.44516 (8)	0.03642 (6)	0.01504 (17)
H5	0.2750	0.5070	0.0341	0.018*
C6	0.22782 (12)	0.36598 (8)	−0.00374 (6)	0.01598 (18)
C7	0.29217 (13)	0.27321 (9)	−0.00227 (7)	0.01821 (19)
H7	0.2302	0.2211	−0.0305	0.022*
C8	0.45046 (13)	0.25954 (9)	0.04208 (7)	0.01821 (19)
H8	0.4942	0.1974	0.0438	0.022*
C9	0.54584 (12)	0.33745 (8)	0.08428 (6)	0.01469 (17)
C10	0.80650 (12)	0.40097 (8)	0.15527 (6)	0.01407 (17)
H10	0.8271	0.4245	0.1147	0.017*
C11	0.95981 (12)	0.38117 (8)	0.22454 (6)	0.01524 (17)
H11	0.9365	0.3457	0.2607	0.018*
C12	0.97389 (13)	0.48916 (9)	0.37889 (7)	0.01797 (19)
C13	0.93661 (13)	0.39511 (9)	0.39459 (7)	0.0197 (2)
H13	0.9872	0.3392	0.3891	0.024*
C14	0.82254 (14)	0.38560 (11)	0.41864 (7)	0.0231 (2)
H14	0.7998	0.3231	0.4308	0.028*
C15	0.74214 (15)	0.46833 (12)	0.42474 (7)	0.0246 (2)
C16	0.78110 (17)	0.56192 (12)	0.40851 (8)	0.0274 (3)
H16	0.7283	0.6177	0.4125	0.033*
C17	0.89758 (16)	0.57311 (10)	0.38651 (8)	0.0233 (2)
H17	0.9244	0.6360	0.3770	0.028*
C18	0.61530 (19)	0.45797 (15)	0.44829 (10)	0.0352 (3)
H18A	0.6093	0.3901	0.4613	0.053*
H18B	0.5175	0.4774	0.4081	0.053*
H18C	0.6382	0.4998	0.4904	0.053*
C19	0.51164 (12)	0.59192 (8)	0.15662 (6)	0.01492 (18)
C20	0.53584 (13)	0.69413 (9)	0.15655 (7)	0.0195 (2)
H20	0.5836	0.7198	0.1293	0.023*
C21	0.48931 (15)	0.75812 (10)	0.19693 (8)	0.0268 (3)
H21	0.5076	0.8260	0.1971	0.032*
C22	0.41570 (16)	0.72071 (12)	0.23691 (8)	0.0295 (3)
H22	0.3846	0.7634	0.2639	0.035*
C23	0.38881 (16)	0.61938 (12)	0.23646 (8)	0.0281 (3)
H23	0.3378	0.5943	0.2624	0.034*

C24	0.43787 (14)	0.55503 (10)	0.19723 (7)	0.0213 (2)
H24	0.4214	0.4870	0.1981	0.026*
C25	1.08137 (13)	0.32202 (9)	0.21256 (7)	0.0192 (2)
H25A	1.1749	0.3178	0.2595	0.023*
H25B	1.0426	0.2549	0.1982	0.023*
C26	1.12569 (16)	0.36324 (11)	0.15477 (9)	0.0265 (3)
H26A	1.2025	0.3210	0.1513	0.040*
H26B	1.1676	0.4289	0.1689	0.040*
H26C	1.0350	0.3659	0.1075	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01395 (4)	0.02093 (5)	0.01897 (6)	−0.00094 (4)	0.00462 (4)	−0.00109 (4)
S1	0.01233 (9)	0.01608 (11)	0.01730 (12)	−0.00234 (8)	0.00355 (8)	0.00071 (9)
O1	0.0193 (4)	0.0188 (4)	0.0239 (5)	−0.0068 (3)	0.0058 (3)	−0.0019 (3)
O2	0.0137 (3)	0.0224 (4)	0.0233 (4)	0.0014 (3)	0.0031 (3)	0.0035 (3)
N1	0.0130 (3)	0.0142 (4)	0.0165 (4)	0.0004 (3)	0.0046 (3)	0.0013 (3)
N2	0.0143 (3)	0.0113 (4)	0.0230 (5)	0.0005 (3)	0.0068 (3)	−0.0021 (3)
C1	0.0139 (4)	0.0123 (4)	0.0172 (5)	−0.0001 (3)	0.0057 (3)	0.0005 (3)
C2	0.0128 (3)	0.0117 (4)	0.0150 (4)	0.0002 (3)	0.0064 (3)	−0.0001 (3)
C3	0.0136 (4)	0.0126 (4)	0.0143 (4)	0.0000 (3)	0.0067 (3)	−0.0001 (3)
C4	0.0140 (4)	0.0128 (4)	0.0137 (4)	−0.0004 (3)	0.0068 (3)	−0.0002 (3)
C5	0.0151 (4)	0.0150 (4)	0.0150 (5)	0.0005 (3)	0.0067 (3)	0.0001 (3)
C6	0.0140 (4)	0.0170 (5)	0.0155 (5)	−0.0018 (3)	0.0054 (3)	−0.0011 (4)
C7	0.0172 (4)	0.0156 (4)	0.0199 (5)	−0.0028 (3)	0.0067 (4)	−0.0028 (4)
C8	0.0176 (4)	0.0133 (4)	0.0218 (5)	−0.0011 (3)	0.0072 (4)	−0.0024 (4)
C9	0.0147 (4)	0.0131 (4)	0.0163 (5)	0.0001 (3)	0.0070 (3)	0.0000 (3)
C10	0.0128 (4)	0.0126 (4)	0.0166 (5)	0.0002 (3)	0.0064 (3)	−0.0001 (3)
C11	0.0141 (4)	0.0133 (4)	0.0172 (5)	0.0001 (3)	0.0061 (3)	0.0009 (4)
C12	0.0157 (4)	0.0206 (5)	0.0148 (5)	−0.0023 (3)	0.0045 (4)	0.0004 (4)
C13	0.0157 (4)	0.0215 (5)	0.0183 (5)	−0.0002 (3)	0.0045 (4)	0.0045 (4)
C14	0.0195 (5)	0.0283 (6)	0.0191 (5)	−0.0039 (4)	0.0068 (4)	0.0039 (5)
C15	0.0231 (5)	0.0342 (7)	0.0169 (5)	−0.0046 (5)	0.0094 (4)	−0.0031 (5)
C16	0.0328 (6)	0.0282 (7)	0.0260 (7)	−0.0002 (5)	0.0176 (5)	−0.0061 (5)
C17	0.0300 (6)	0.0197 (5)	0.0228 (6)	−0.0022 (4)	0.0141 (5)	−0.0038 (4)
C18	0.0327 (7)	0.0498 (10)	0.0309 (8)	−0.0065 (6)	0.0212 (6)	−0.0053 (7)
C19	0.0133 (4)	0.0147 (4)	0.0157 (5)	0.0018 (3)	0.0056 (3)	−0.0021 (3)
C20	0.0185 (4)	0.0152 (5)	0.0220 (6)	0.0024 (3)	0.0067 (4)	−0.0019 (4)
C21	0.0241 (5)	0.0196 (5)	0.0304 (7)	0.0064 (4)	0.0067 (5)	−0.0080 (5)
C22	0.0244 (5)	0.0361 (7)	0.0248 (6)	0.0097 (5)	0.0084 (5)	−0.0108 (5)
C23	0.0251 (5)	0.0393 (8)	0.0240 (6)	0.0039 (5)	0.0146 (5)	−0.0052 (6)
C24	0.0210 (5)	0.0242 (6)	0.0216 (6)	0.0001 (4)	0.0123 (4)	−0.0023 (4)
C25	0.0162 (4)	0.0161 (5)	0.0244 (6)	0.0032 (3)	0.0083 (4)	0.0012 (4)
C26	0.0230 (5)	0.0265 (6)	0.0361 (8)	0.0056 (4)	0.0188 (5)	0.0046 (5)

Geometric parameters (Å, º)

Br1—C6	1.9048 (11)	C12—C13	1.3909 (17)
S1—O2	1.4363 (10)	C12—C17	1.3937 (19)
S1—O1	1.4392 (9)	C13—C14	1.3940 (18)
S1—N1	1.6375 (10)	C13—H13	0.93
S1—C12	1.7619 (12)	C14—C15	1.393 (2)
N1—C1	1.5025 (14)	C14—H14	0.93
N1—C11	1.5083 (15)	C15—C16	1.395 (2)
N2—C9	1.3930 (14)	C15—C18	1.505 (2)
N2—C10	1.4408 (14)	C16—C17	1.389 (2)
N2—H1N2	0.83 (2)	C16—H16	0.93
C1—C2	1.5239 (14)	C17—H17	0.93
C1—H1A	0.97	C18—H18A	0.96
C1—H1B	0.97	C18—H18B	0.96
C2—C10	1.5140 (15)	C18—H18C	0.96
C2—C3	1.5260 (14)	C19—C20	1.3952 (16)
C2—H2	0.98	C19—C24	1.3976 (17)
C3—C19	1.5171 (15)	C20—C21	1.3929 (18)
C3—C4	1.5306 (15)	C20—H20	0.93
C3—H3	0.98	C21—C22	1.389 (2)
C4—C5	1.4006 (14)	C21—H21	0.93
C4—C9	1.4145 (15)	C22—C23	1.387 (2)
C5—C6	1.3898 (15)	C22—H22	0.93
C5—H5	0.93	C23—C24	1.3933 (19)
C6—C7	1.3881 (17)	C23—H23	0.93
C7—C8	1.3867 (16)	C24—H24	0.93
C7—H7	0.93	C25—C26	1.5188 (19)
C8—C9	1.4003 (16)	C25—H25A	0.97
C8—H8	0.93	C25—H25B	0.97
C10—C11	1.5294 (15)	C26—H26A	0.96
C10—H10	0.98	C26—H26B	0.96
C11—C25	1.5230 (16)	C26—H26C	0.96
C11—H11	0.98		

O2—S1—O1	119.64 (6)	N1—C11—H11	108.4
O2—S1—N1	106.93 (6)	C25—C11—H11	108.4
O1—S1—N1	106.70 (6)	C10—C11—H11	108.4
O2—S1—C12	108.58 (6)	C13—C12—C17	120.60 (12)
O1—S1—C12	107.56 (6)	C13—C12—S1	119.32 (10)
N1—S1—C12	106.77 (5)	C17—C12—S1	119.91 (10)
C1—N1—C11	109.52 (8)	C12—C13—C14	119.25 (12)
C1—N1—S1	114.59 (8)	C12—C13—H13	120.4
C11—N1—S1	117.20 (8)	C14—C13—H13	120.4
C9—N2—C10	116.82 (9)	C15—C14—C13	120.98 (12)
C9—N2—H1N2	117.8 (13)	C15—C14—H14	119.5
C10—N2—H1N2	117.2 (13)	C13—C14—H14	119.5
N1—C1—C2	102.39 (8)	C14—C15—C16	118.77 (12)

N1—C1—H1A	111.3	C14—C15—C18	121.14 (14)
C2—C1—H1A	111.3	C16—C15—C18	120.09 (14)
N1—C1—H1B	111.3	C17—C16—C15	121.01 (13)
C2—C1—H1B	111.3	C17—C16—H16	119.5
H1A—C1—H1B	109.2	C15—C16—H16	119.5
C10—C2—C1	100.61 (8)	C16—C17—C12	119.34 (13)
C10—C2—C3	113.45 (9)	C16—C17—H17	120.3
C1—C2—C3	118.62 (9)	C12—C17—H17	120.3
C10—C2—H2	107.9	C15—C18—H18A	109.5
C1—C2—H2	107.9	C15—C18—H18B	109.5
C3—C2—H2	107.9	H18A—C18—H18B	109.5
C19—C3—C2	108.23 (9)	C15—C18—H18C	109.5
C19—C3—C4	115.39 (9)	H18A—C18—H18C	109.5
C2—C3—C4	108.39 (9)	H18B—C18—H18C	109.5
C19—C3—H3	108.2	C20—C19—C24	118.71 (11)
C2—C3—H3	108.2	C20—C19—C3	119.97 (10)
C4—C3—H3	108.2	C24—C19—C3	120.91 (10)
C5—C4—C9	118.53 (10)	C21—C20—C19	120.71 (13)
C5—C4—C3	119.87 (9)	C21—C20—H20	119.6
C9—C4—C3	121.58 (9)	C19—C20—H20	119.6
C6—C5—C4	120.63 (10)	C22—C21—C20	120.10 (13)
C6—C5—H5	119.7	C22—C21—H21	120.0
C4—C5—H5	119.7	C20—C21—H21	120.0
C7—C6—C5	121.05 (10)	C23—C22—C21	119.70 (12)
C7—C6—Br1	118.84 (8)	C23—C22—H22	120.1
C5—C6—Br1	120.10 (8)	C21—C22—H22	120.1
C8—C7—C6	118.84 (10)	C22—C23—C24	120.29 (14)
C8—C7—H7	120.6	C22—C23—H23	119.9
C6—C7—H7	120.6	C24—C23—H23	119.9
C7—C8—C9	121.34 (11)	C23—C24—C19	120.47 (13)
C7—C8—H8	119.3	C23—C24—H24	119.8
C9—C8—H8	119.3	C19—C24—H24	119.8
N2—C9—C8	118.47 (10)	C26—C25—C11	115.82 (10)
N2—C9—C4	121.95 (10)	C26—C25—H25A	108.3
C8—C9—C4	119.54 (10)	C11—C25—H25A	108.3
N2—C10—C2	109.73 (9)	C26—C25—H25B	108.3
N2—C10—C11	114.21 (9)	C11—C25—H25B	108.3
C2—C10—C11	101.94 (9)	H25A—C25—H25B	107.4
N2—C10—H10	110.2	C25—C26—H26A	109.5
C2—C10—H10	110.2	C25—C26—H26B	109.5
C11—C10—H10	110.2	H26A—C26—H26B	109.5
N1—C11—C25	114.16 (9)	C25—C26—H26C	109.5
N1—C11—C10	101.06 (8)	H26A—C26—H26C	109.5
C25—C11—C10	115.98 (10)	H26B—C26—H26C	109.5

O2—S1—N1—C1	171.86 (8)	C1—N1—C11—C25	140.52 (10)
O1—S1—N1—C1	−59.00 (9)	S1—N1—C11—C25	−86.74 (11)
C12—S1—N1—C1	55.78 (9)	C1—N1—C11—C10	15.29 (11)

O2—S1—N1—C11	41.45 (9)	S1—N1—C11—C10	148.03 (8)
O1—S1—N1—C11	170.58 (8)	N2—C10—C11—N1	−158.08 (9)
C12—S1—N1—C11	−74.64 (9)	C2—C10—C11—N1	−39.82 (10)
C11—N1—C1—C2	14.81 (12)	N2—C10—C11—C25	77.92 (13)
S1—N1—C1—C2	−119.27 (8)	C2—C10—C11—C25	−163.81 (9)
N1—C1—C2—C10	−39.19 (10)	O2—S1—C12—C13	−30.53 (11)
N1—C1—C2—C3	−163.49 (9)	O1—S1—C12—C13	−161.35 (9)
C10—C2—C3—C19	171.06 (9)	N1—S1—C12—C13	84.45 (10)
C1—C2—C3—C19	−71.20 (12)	O2—S1—C12—C17	154.32 (10)
C10—C2—C3—C4	45.25 (12)	O1—S1—C12—C17	23.50 (12)
C1—C2—C3—C4	162.98 (9)	N1—S1—C12—C17	−90.71 (11)
C19—C3—C4—C5	41.53 (14)	C17—C12—C13—C14	−0.47 (18)
C2—C3—C4—C5	163.04 (10)	S1—C12—C13—C14	−175.59 (9)
C19—C3—C4—C9	−140.35 (11)	C12—C13—C14—C15	2.16 (19)
C2—C3—C4—C9	−18.85 (14)	C13—C14—C15—C16	−2.0 (2)
C9—C4—C5—C6	−1.42 (17)	C13—C14—C15—C18	177.98 (13)
C3—C4—C5—C6	176.75 (10)	C14—C15—C16—C17	0.1 (2)
C4—C5—C6—C7	−0.96 (18)	C18—C15—C16—C17	−179.85 (14)
C4—C5—C6—Br1	178.88 (9)	C15—C16—C17—C12	1.5 (2)
C5—C6—C7—C8	2.08 (19)	C13—C12—C17—C16	−1.4 (2)
Br1—C6—C7—C8	−177.76 (10)	S1—C12—C17—C16	173.74 (11)
C6—C7—C8—C9	−0.81 (19)	C2—C3—C19—C20	95.33 (12)
C10—N2—C9—C8	160.86 (11)	C4—C3—C19—C20	−143.08 (11)
C10—N2—C9—C4	−21.63 (16)	C2—C3—C19—C24	−77.22 (12)
C7—C8—C9—N2	176.02 (11)	C4—C3—C19—C24	44.37 (14)
C7—C8—C9—C4	−1.56 (18)	C24—C19—C20—C21	0.84 (17)
C5—C4—C9—N2	−174.85 (11)	C3—C19—C20—C21	−171.88 (11)
C3—C4—C9—N2	7.01 (17)	C19—C20—C21—C22	−1.04 (19)
C5—C4—C9—C8	2.64 (17)	C20—C21—C22—C23	0.0 (2)
C3—C4—C9—C8	−175.50 (11)	C21—C22—C23—C24	1.2 (2)
C9—N2—C10—C2	47.11 (14)	C22—C23—C24—C19	−1.4 (2)
C9—N2—C10—C11	160.83 (10)	C20—C19—C24—C23	0.37 (18)
C1—C2—C10—N2	171.23 (9)	C3—C19—C24—C23	173.02 (11)
C3—C2—C10—N2	−61.01 (12)	N1—C11—C25—C26	−62.22 (14)
C1—C2—C10—C11	49.81 (10)	C10—C11—C25—C26	54.68 (14)
C3—C2—C10—C11	177.58 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1*N*2···O1^{i}	0.83 (2)	2.33 (2)	3.1381 (14)	162 (2)
C25—H25*A*···O2	0.97	2.49	3.1312 (15)	123
C3—H3···*Cg*1^{ii}	0.98	2.83	3.7921 (12)	168

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