organic compounds

7-Chloro-3-ethyl-10-phenyl-2-tosyl-pyrrolo[3,4-b]quinoline

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The pyrrolidine ring of the title molecule, $C_{26}H_{27}ClN_2O_2S$, adopts a twist conformation, while the tetrahydropyridine ring is in a half-chair conformation. The tosyl group is attached to the pyrrolidine ring in a biaxial position. The pyrrolidine and tetrahydropyridine rings are *trans*-fused. The pyridine-fused benzene ring forms dihedral angles of 73.95 (2) and 19.18 (5)°, respectively, with the benzene ring of the chlorobenzene and tosyl groups. The screw-related molecules are linked into a chain along the [010] direction by N—H···O hydrogen bonds, and the chains are cross-linked into a three-dimensional network by C—H···π interactions and weak π–π interactions [centroid–centroid distance = 3.7488 (5) Å].

Related literature

For general background, see: Anzini *et al.* (1990, 1992); Crenshaw *et al.* (1976); Fujita *et al.* (1996); Xiao *et al.* (2006). For a related structure, see: Sudha *et al.* (2007). For ring-puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Duax *et al.* (1976). For bond-length data, see: Allen *et al.* (1987).
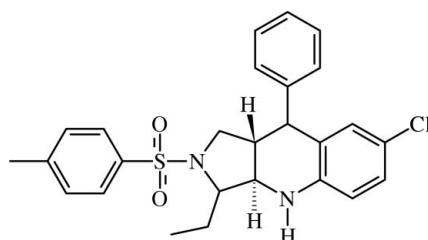
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Experimental

Crystal data

$C_{26}H_{27}ClN_2O_2S$	V = 2321.91 (7) Å³
M_r = 467.01	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 9.5843 (2) Å	μ = 0.28 mm⁻¹
b = 13.2007 (2) Å	T = 100.0 (1) K
c = 20.3414 (3) Å	0.50 × 0.41 × 0.40 mm
β = 115.550 (1)°	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	115565 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	14373 independent reflections
	11857 reflections with $I > 2\sigma(I)$
T_{min} = 0.780, T_{max} = 0.897	R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.109	
S = 1.03	
14373 reflections	$\Delta\rho_{max}$ = 0.61 e Å⁻³
294 parameters	$\Delta\rho_{min}$ = −0.42 e Å⁻³

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

$Cg1$ is the centroid of the C4–C9 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1N2···O1[i]	0.829 (14)	2.358 (14)	3.1454 (8)	159 (2)
C25—H25B···O2	0.97	2.51	3.1399 (9)	123
C3—H3···$Cg1$[ii]	0.98	2.85	3.7962 (8)	163

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

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 materials

7-Chloro-3-ethyl-10-phenyl-2-tosylpyrrolo[3,4-*b*]quinoline

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Comment

Pyrrolo[3,4-*b*]quinoline derivatives exhibit cytotoxic (Xiao *et al.*, 2006), antibacterial (Fujita *et al.*, 1996) and interferon inducing activities (Crenshaw *et al.*, 1976). They are also found to bind benzodiazepine receptors (Anzini *et al.*, 1990, 1992). Previously, we have reported the crystal structure of a pyrrolo[3,4-*b*]quinoline derivative (Sudha *et al.*, 2007). We report herein the crystal structure of the title pyrroloquinoline derivative, (I), Fig. 1.

Bond lengths and angles show normal values (Allen *et al.*, 1987), and are comparable with those in a related structure (Sudha *et al.*, 2007). As a result of the repulsive interaction between the short S═O bonds, atom S1 has a distorted tetrahedral configuration, with the O2—S1—O1 [119.63 (4)°] angle deviating significantly from ideal tetrahedral value.

The pyrrolidine ring has a twist conformation, with the local twofold rotation axis passes through atom N1 and the midpoint of the bond C2—C10. The relevant asymmetry parameters ΔC_2[C2—C10] (Duax *et al.*, 1976) and the puckering parameters q_2 and φ (Cremer & Pople, 1975) are 0.24 (7)°, 0.4686 (8) Å and 90.05 (9)°, respectively. The tosyl group is attached to the pyrrolidine ring in a biaxial position.

The tetrahydropyridine ring adopts a half-chair conformation with a local twofold rotation axis passing through the midpoints of the C4—C9 and C2—C10 bonds; the puckering (Q, θ, φ) and asymmetry (ΔC_2[C4—C9]) parameters are 0.4744 (8) Å, 133.81 (10)°, 89.08 (13)° and 2.29 (10)°, respectively. The pyrrolidine and tetrahydropyridine rings are *trans*-fused. The C19—C24 phenyl ring forms dihedral angles of 73.95 (2) and 19.18 (5)°, respectively, with the C4—C9 and C12—C17 benzene rings.

The screw-related molecules are linked into a chain along the [0 1 0] direction by N—H···O hydrogen bonds. The chains are cross-linked into a three-dimensional network (Fig.2) by C—H···π interactions involving the C3—H3 group and the C4—C9 benzene ring (centroid *Cg*1) of the molecule at ($-x$, $1 - y$, $-z$), and π-π interactions between the C12—C17 benzene rings of molecules at (x, y, z) and ($1 - x$, $1 - y$, $1 - z$) [centroid-centroid distance is 3.7488 (5) Å].

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 (2o 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$_2$SO$_4$. 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.

supplementary materials

Refinement

The N-bound H atom was located from a difference map and refined freely with an isotropic displacement parameter. 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.

Figures
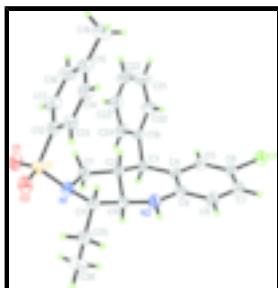
Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 80% probability level.
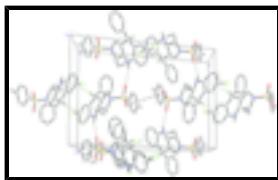
Fig. 2. Part of the three-dimensional network in the title compound. Dashed and dotted lines indicate N—H···O and C—H···π interactions, respectively. The π-π interaction is shown by a dashed open line. For the sake of clarity, H atoms not involved in the interactions have been omitted.

7-Chloro-3-ethyl-10-phenyl-2-tosylpyrrolo[3,4-*b*]quinoline

Crystal data

$C_{26}H_{27}ClN_2O_2S$	$F_{000} = 984$
$M_r = 467.01$	$D_x = 1.336$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 9717 reflections
$a = 9.5843$ (2) Å	$\theta = 2.4$–41.9º
$b = 13.2007$ (2) Å	$\mu = 0.28$ mm^{-1}
$c = 20.3414$ (3) Å	$T = 100.0$ (1) K
$\beta = 115.550$ (1)º	Block, colourless
$V = 2321.91$ (7) Å^3	$0.50 \times 0.41 \times 0.40$ mm
$Z = 4$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	14373 independent reflections
Radiation source: fine-focus sealed tube	11857 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.043$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 40.0$º

$T = 100.0(1)$ K	$\theta_{min} = 2.2°$
ω scans	$h = -17 \rightarrow 17$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$k = -23 \rightarrow 23$
$T_{min} = 0.780$, $T_{max} = 0.897$	$l = -36 \rightarrow 36$
115565 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.109$	$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.4777P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
14373 reflections	$\Delta\rho_{max} = 0.61$ e Å^{-3}
294 parameters	$\Delta\rho_{min} = -0.42$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2sigma(F^2)$ 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*	$U_{iso}*/U_{eq}$
Cl1	−0.46322 (2)	0.604543 (14)	−0.054121 (10)	0.01947 (4)
S1	0.61137 (2)	0.510831 (13)	0.338265 (10)	0.01478 (4)
O1	0.66669 (7)	0.40806 (4)	0.35158 (3)	0.02040 (10)
O2	0.72013 (7)	0.59313 (4)	0.36178 (3)	0.01988 (10)
N1	0.51131 (7)	0.52196 (4)	0.25005 (3)	0.01442 (9)
N2	0.20015 (7)	0.68671 (4)	0.12988 (4)	0.01623 (10)
H1N2	0.2303 (16)	0.7428 (10)	0.1229 (8)	0.028 (3)*
C1	0.37966 (8)	0.44894 (5)	0.21613 (4)	0.01491 (10)
H1A	0.3709	0.4054	0.2526	0.018*
H1B	0.3917	0.4073	0.1796	0.018*

C2	0.24059 (8)	0.51861 (5)	0.18181 (4)	0.01314 (10)
H2	0.2183	0.5463	0.2210	0.016*
C3	0.09024 (8)	0.47624 (5)	0.12322 (4)	0.01293 (10)
H3	0.1152	0.4373	0.0887	0.016*
C4	−0.01388 (8)	0.56469 (5)	0.08214 (4)	0.01342 (10)
C5	−0.17147 (8)	0.54847 (5)	0.03904 (4)	0.01475 (10)
H5	−0.2130	0.4843	0.0371	0.018*
C6	−0.26683 (8)	0.62687 (5)	−0.00093 (4)	0.01552 (10)
C7	−0.20779 (9)	0.72344 (5)	0.00073 (4)	0.01768 (11)
H7	−0.2718	0.7755	−0.0268	0.021*
C8	−0.05244 (9)	0.74104 (5)	0.04386 (4)	0.01753 (11)
H8	−0.0128	0.8058	0.0455	0.021*
C9	0.04660 (8)	0.66348 (5)	0.08514 (4)	0.01436 (10)
C10	0.30748 (8)	0.60324 (5)	0.15364 (4)	0.01342 (10)
H10	0.3284	0.5787	0.1133	0.016*
C11	0.45891 (8)	0.62662 (5)	0.21984 (4)	0.01418 (10)
H11	0.4354	0.6651	0.2550	0.017*
C12	0.48094 (8)	0.52634 (5)	0.37754 (4)	0.01599 (11)
C13	0.44059 (9)	0.62360 (6)	0.39012 (4)	0.01736 (11)
H13	0.4866	0.6801	0.3804	0.021*
C14	0.33104 (9)	0.63518 (6)	0.41731 (4)	0.02117 (13)
H14	0.3060	0.6999	0.4268	0.025*
C15	0.25807 (10)	0.55165 (7)	0.43055 (5)	0.02340 (14)
C16	0.30038 (11)	0.45522 (7)	0.41780 (5)	0.02539 (15)
H16	0.2529	0.3988	0.4266	0.030*
C17	0.41188 (10)	0.44177 (6)	0.39219 (5)	0.02144 (13)
H17	0.4403	0.3769	0.3849	0.026*
C18	0.13611 (13)	0.56452 (10)	0.45801 (6)	0.0352 (2)
H18A	0.1420	0.6317	0.4770	0.053*
H18B	0.1529	0.5160	0.4958	0.053*
H18C	0.0357	0.5540	0.4187	0.053*
C19	0.02137 (8)	0.40411 (5)	0.15955 (4)	0.01436 (10)
C20	−0.05309 (10)	0.44085 (6)	0.20051 (5)	0.02128 (13)
H20	−0.0713	0.5100	0.2011	0.026*
C21	−0.10042 (12)	0.37489 (8)	0.24045 (5)	0.02782 (17)
H21	−0.1509	0.4000	0.2671	0.033*
C22	−0.07219 (11)	0.27164 (7)	0.24043 (5)	0.02752 (17)
H22	−0.1026	0.2276	0.2675	0.033*
C23	0.00145 (10)	0.23441 (6)	0.19981 (5)	0.02406 (15)
H23	0.0206	0.1653	0.1998	0.029*
C24	0.04692 (9)	0.30017 (5)	0.15897 (4)	0.01788 (12)
H24	0.0946	0.2745	0.1312	0.021*
C25	0.57811 (9)	0.68532 (5)	0.20407 (4)	0.01726 (11)
H25A	0.5364	0.7520	0.1863	0.021*
H25B	0.6696	0.6946	0.2496	0.021*
C26	0.62696 (10)	0.63715 (7)	0.14935 (5)	0.02466 (15)
H26A	0.7018	0.6797	0.1432	0.037*
H26B	0.5382	0.6295	0.1034	0.037*
H26C	0.6717	0.5719	0.1669	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.01587 (7)	0.02092 (8)	0.01830 (8)	0.00043 (5)	0.00424 (6)	0.00035 (5)
S1	0.01325 (7)	0.01446 (7)	0.01487 (7)	0.00160 (5)	0.00440 (6)	0.00037 (5)
O1	0.0208 (3)	0.0166 (2)	0.0214 (3)	0.00656 (18)	0.0068 (2)	0.00265 (18)
O2	0.0148 (2)	0.0208 (2)	0.0205 (3)	−0.00274 (17)	0.00431 (19)	−0.00168 (18)
N1	0.0147 (2)	0.0130 (2)	0.0143 (2)	−0.00002 (16)	0.00514 (19)	0.00044 (17)
N2	0.0149 (2)	0.0112 (2)	0.0212 (3)	0.00013 (17)	0.0065 (2)	0.00268 (18)
C1	0.0153 (3)	0.0122 (2)	0.0156 (3)	0.00003 (18)	0.0051 (2)	0.00010 (19)
C2	0.0144 (2)	0.0116 (2)	0.0139 (3)	−0.00003 (17)	0.0066 (2)	0.00053 (18)
C3	0.0144 (2)	0.0116 (2)	0.0138 (3)	0.00027 (17)	0.0069 (2)	0.00067 (17)
C4	0.0153 (2)	0.0124 (2)	0.0134 (3)	0.00074 (18)	0.0070 (2)	0.00097 (18)
C5	0.0157 (3)	0.0143 (2)	0.0140 (3)	0.00022 (19)	0.0061 (2)	0.00023 (19)
C6	0.0151 (3)	0.0168 (3)	0.0140 (3)	0.0015 (2)	0.0057 (2)	0.00011 (19)
C7	0.0176 (3)	0.0153 (3)	0.0186 (3)	0.0028 (2)	0.0064 (2)	0.0023 (2)
C8	0.0179 (3)	0.0130 (2)	0.0207 (3)	0.0017 (2)	0.0074 (2)	0.0030 (2)
C9	0.0152 (3)	0.0128 (2)	0.0155 (3)	0.00094 (18)	0.0070 (2)	0.00149 (19)
C10	0.0138 (2)	0.0120 (2)	0.0150 (3)	0.00031 (17)	0.0067 (2)	0.00106 (18)
C11	0.0155 (3)	0.0119 (2)	0.0153 (3)	0.00014 (18)	0.0068 (2)	−0.00002 (18)
C12	0.0169 (3)	0.0163 (3)	0.0139 (3)	0.0006 (2)	0.0057 (2)	−0.00019 (19)
C13	0.0165 (3)	0.0177 (3)	0.0160 (3)	0.0007 (2)	0.0053 (2)	−0.0019 (2)
C14	0.0194 (3)	0.0259 (3)	0.0173 (3)	0.0043 (2)	0.0071 (3)	−0.0017 (2)
C15	0.0203 (3)	0.0348 (4)	0.0162 (3)	0.0023 (3)	0.0088 (3)	0.0020 (3)
C16	0.0287 (4)	0.0283 (4)	0.0234 (4)	−0.0031 (3)	0.0153 (3)	0.0034 (3)
C17	0.0277 (4)	0.0185 (3)	0.0206 (3)	−0.0011 (2)	0.0128 (3)	0.0013 (2)
C18	0.0286 (4)	0.0551 (6)	0.0287 (5)	0.0069 (4)	0.0188 (4)	0.0065 (4)
C19	0.0141 (2)	0.0144 (2)	0.0146 (3)	−0.00066 (18)	0.0062 (2)	0.00182 (19)
C20	0.0241 (3)	0.0225 (3)	0.0228 (3)	0.0006 (2)	0.0153 (3)	0.0021 (2)
C21	0.0289 (4)	0.0359 (4)	0.0258 (4)	−0.0038 (3)	0.0185 (4)	0.0036 (3)
C22	0.0257 (4)	0.0325 (4)	0.0236 (4)	−0.0088 (3)	0.0098 (3)	0.0085 (3)
C23	0.0238 (4)	0.0187 (3)	0.0255 (4)	−0.0052 (2)	0.0066 (3)	0.0064 (3)
C24	0.0181 (3)	0.0143 (2)	0.0198 (3)	−0.0016 (2)	0.0068 (2)	0.0021 (2)
C25	0.0173 (3)	0.0151 (3)	0.0194 (3)	−0.0031 (2)	0.0079 (2)	−0.0008 (2)
C26	0.0233 (4)	0.0272 (4)	0.0296 (4)	−0.0060 (3)	0.0172 (3)	−0.0048 (3)

Geometric parameters (Å, °)

Cl1—C6	1.7447 (7)	C12—C17	1.3941 (11)
S1—O2	1.4373 (6)	C12—C13	1.3959 (10)
S1—O1	1.4392 (6)	C13—C14	1.3902 (11)
S1—N1	1.6360 (6)	C13—H13	0.93
S1—C12	1.7619 (7)	C14—C15	1.3928 (13)
N1—C1	1.4988 (9)	C14—H14	0.93
N1—C11	1.5075 (9)	C15—C16	1.3938 (13)
N2—C9	1.3902 (9)	C15—C18	1.5069 (12)
N2—C10	1.4412 (9)	C16—C17	1.3875 (12)
N2—H1N2	0.830 (14)	C16—H16	0.93

supplementary materials

C1—C2	1.5189 (9)	C17—H17	0.93
C1—H1A	0.97	C18—H18A	0.96
C1—H1B	0.97	C18—H18B	0.96
C2—C10	1.5179 (9)	C18—H18C	0.96
C2—C3	1.5258 (10)	C19—C24	1.3947 (10)
C2—H2	0.98	C19—C20	1.3970 (10)
C3—C19	1.5196 (9)	C20—C21	1.3936 (11)
C3—C4	1.5291 (9)	C20—H20	0.93
C3—H3	0.98	C21—C22	1.3896 (14)
C4—C5	1.3977 (10)	C21—H21	0.93
C4—C9	1.4177 (9)	C22—C23	1.3875 (14)
C5—C6	1.3881 (10)	C22—H22	0.93
C5—H5	0.93	C23—C24	1.3950 (11)
C6—C7	1.3892 (10)	C23—H23	0.93
C7—C8	1.3833 (11)	C24—H24	0.93
C7—H7	0.93	C25—C26	1.5205 (11)
C8—C9	1.4025 (10)	C25—H25A	0.97
C8—H8	0.93	C25—H25B	0.97
C10—C11	1.5262 (10)	C26—H26A	0.96
C10—H10	0.98	C26—H26B	0.96
C11—C25	1.5247 (9)	C26—H26C	0.96
C11—H11	0.98		
O2—S1—O1	119.63 (4)	N1—C11—H11	108.6
O2—S1—N1	107.16 (3)	C25—C11—H11	108.6
O1—S1—N1	106.57 (3)	C10—C11—H11	108.6
O2—S1—C12	108.41 (4)	C17—C12—C13	120.18 (7)
O1—S1—C12	107.47 (4)	C17—C12—S1	119.93 (6)
N1—S1—C12	106.98 (3)	C13—C12—S1	119.79 (5)
C1—N1—C11	109.60 (5)	C14—C13—C12	119.38 (7)
C1—N1—S1	115.22 (5)	C14—C13—H13	120.3
C11—N1—S1	117.65 (5)	C12—C13—H13	120.3
C9—N2—C10	116.86 (6)	C13—C14—C15	121.21 (7)
C9—N2—H1N2	115.7 (10)	C13—C14—H14	119.4
C10—N2—H1N2	119.3 (10)	C15—C14—H14	119.4
N1—C1—C2	102.70 (5)	C14—C15—C16	118.45 (7)
N1—C1—H1A	111.2	C14—C15—C18	121.13 (9)
C2—C1—H1A	111.2	C16—C15—C18	120.42 (9)
N1—C1—H1B	111.2	C17—C16—C15	121.31 (8)
C2—C1—H1B	111.2	C17—C16—H16	119.3
H1A—C1—H1B	109.1	C15—C16—H16	119.3
C10—C2—C1	100.92 (5)	C16—C17—C12	119.43 (8)
C10—C2—C3	112.66 (6)	C16—C17—H17	120.3
C1—C2—C3	118.88 (5)	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	108.17 (5)	C15—C18—H18C	109.5
C19—C3—C4	115.23 (5)	H18A—C18—H18C	109.5
C2—C3—C4	108.71 (5)	H18B—C18—H18C	109.5

C19—C3—H3	108.2	C24—C19—C20	118.91 (6)
C2—C3—H3	108.2	C24—C19—C3	119.84 (6)
C4—C3—H3	108.2	C20—C19—C3	120.88 (6)
C5—C4—C9	118.63 (6)	C21—C20—C19	120.61 (8)
C5—C4—C3	119.98 (6)	C21—C20—H20	119.7
C9—C4—C3	121.37 (6)	C19—C20—H20	119.7
C6—C5—C4	120.90 (6)	C22—C21—C20	120.01 (8)
C6—C5—H5	119.5	C22—C21—H21	120.0
C4—C5—H5	119.5	C20—C21—H21	120.0
C5—C6—C7	120.77 (7)	C23—C22—C21	119.79 (7)
C5—C6—Cl1	119.93 (5)	C23—C22—H22	120.1
C7—C6—Cl1	119.30 (6)	C21—C22—H22	120.1
C8—C7—C6	119.03 (7)	C22—C23—C24	120.27 (8)
C8—C7—H7	120.5	C22—C23—H23	119.9
C6—C7—H7	120.5	C24—C23—H23	119.9
C7—C8—C9	121.50 (6)	C19—C24—C23	120.40 (7)
C7—C8—H8	119.2	C19—C24—H24	119.8
C9—C8—H8	119.2	C23—C24—H24	119.8
N2—C9—C8	118.88 (6)	C26—C25—C11	115.89 (6)
N2—C9—C4	121.93 (6)	C26—C25—H25A	108.3
C8—C9—C4	119.15 (6)	C11—C25—H25A	108.3
N2—C10—C2	109.44 (5)	C26—C25—H25B	108.3
N2—C10—C11	114.26 (5)	C11—C25—H25B	108.3
C2—C10—C11	102.21 (5)	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	113.80 (6)	C25—C26—H26C	109.5
N1—C11—C10	101.37 (5)	H26A—C26—H26C	109.5
C25—C11—C10	115.53 (6)	H26B—C26—H26C	109.5
O2—S1—N1—C1	−173.83 (5)	C1—N1—C11—C25	−139.26 (6)
O1—S1—N1—C1	56.99 (6)	S1—N1—C11—C25	86.54 (7)
C12—S1—N1—C1	−57.73 (5)	C1—N1—C11—C10	−14.57 (7)
O2—S1—N1—C11	−42.12 (6)	S1—N1—C11—C10	−148.77 (5)
O1—S1—N1—C11	−171.30 (5)	N2—C10—C11—N1	156.64 (5)
C12—S1—N1—C11	73.98 (5)	C2—C10—C11—N1	38.54 (6)
C11—N1—C1—C2	−14.91 (7)	N2—C10—C11—C25	−79.85 (7)
S1—N1—C1—C2	120.50 (5)	C2—C10—C11—C25	162.05 (5)
N1—C1—C2—C10	38.47 (6)	O2—S1—C12—C17	−151.08 (7)
N1—C1—C2—C3	162.15 (5)	O1—S1—C12—C17	−20.46 (8)
C10—C2—C3—C19	−171.57 (5)	N1—S1—C12—C17	93.66 (7)
C1—C2—C3—C19	70.74 (7)	O2—S1—C12—C13	32.48 (7)
C10—C2—C3—C4	−45.78 (7)	O1—S1—C12—C13	163.10 (6)
C1—C2—C3—C4	−163.48 (5)	N1—S1—C12—C13	−82.78 (7)
C19—C3—C4—C5	−41.97 (9)	C17—C12—C13—C14	−0.03 (11)
C2—C3—C4—C5	−163.54 (6)	S1—C12—C13—C14	176.40 (6)
C19—C3—C4—C9	139.68 (6)	C12—C13—C14—C15	−1.58 (12)
C2—C3—C4—C9	18.11 (8)	C13—C14—C15—C16	1.74 (13)
C9—C4—C5—C6	0.93 (10)	C13—C14—C15—C18	−178.26 (8)

C3—C4—C5—C6	−177.46 (6)	C14—C15—C16—C17	−0.31 (14)
C4—C5—C6—C7	0.21 (10)	C18—C15—C16—C17	179.69 (9)
C4—C5—C6—Cl1	−179.86 (5)	C15—C16—C17—C12	−1.26 (14)
C5—C6—C7—C8	−1.04 (11)	C13—C12—C17—C16	1.43 (12)
Cl1—C6—C7—C8	179.03 (6)	S1—C12—C17—C16	−175.00 (7)
C6—C7—C8—C9	0.72 (11)	C2—C3—C19—C24	−97.10 (8)
C10—N2—C9—C8	−161.70 (6)	C4—C3—C19—C24	141.03 (7)
C10—N2—C9—C4	20.69 (10)	C2—C3—C19—C20	75.81 (8)
C7—C8—C9—N2	−177.26 (7)	C4—C3—C19—C20	−46.05 (9)
C7—C8—C9—C4	0.42 (11)	C24—C19—C20—C21	0.33 (13)
C5—C4—C9—N2	176.37 (6)	C3—C19—C20—C21	−172.66 (8)
C3—C4—C9—N2	−5.25 (10)	C19—C20—C21—C22	0.70 (15)
C5—C4—C9—C8	−1.23 (10)	C20—C21—C22—C23	−0.80 (15)
C3—C4—C9—C8	177.14 (6)	C21—C22—C23—C24	−0.12 (14)
C9—N2—C10—C2	−47.74 (8)	C20—C19—C24—C23	−1.24 (12)
C9—N2—C10—C11	−161.64 (6)	C3—C19—C24—C23	171.81 (7)
C1—C2—C10—N2	−170.03 (6)	C22—C23—C24—C19	1.15 (13)
C3—C2—C10—N2	62.12 (7)	N1—C11—C25—C26	59.76 (9)
C1—C2—C10—C11	−48.55 (6)	C10—C11—C25—C26	−56.95 (9)
C3—C2—C10—C11	−176.40 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1N2···O1[i]	0.829 (14)	2.358 (14)	3.1454 (8)	159 (2)
C25—H25B···O2	0.97	2.51	3.1399 (9)	123
C3—H3···Cg1[ii]	0.98	2.85	3.7962 (8)	163

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

Fig. 1

Fig. 2