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

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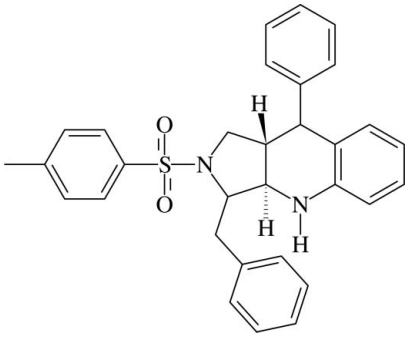
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.045; $wR$ factor = 0.112; data-to-parameter ratio = 19.7.

In the title compound, $C_{31}H_{30}N_2O_2S$, the pyrrolidine ring adopts a twist conformation while the tetrahydropyridine ring is in a half-chair conformation. The two rings are *trans*-fused. The pyridine-bound phenyl ring forms dihedral angles of 17.7 (1) and 48.1 (1)°, respectively, with the tosyl and benzyl phenyl rings. The molecular structure is stabilized by an N—H$\cdots\pi$ interaction involving the benzyl phenyl ring. In the crystal structure, molecules translated by one unit along the *a* axis are linked into chains by C—H$\cdots\pi$ interactions involving the benzene ring of the tosyl group.

## Related literature

For the biological activity of pyrroloquinoline derivatives, see: Ferlin *et al.* (2005); Dalla Via *et al.* (2008); Xiao *et al.* (2006); Fujita *et al.* (1996); Crenshaw *et al.* (1976). For the crystal structure of the 3-ethyl analogue, see: Sudha *et al.* (2008). For ring puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Duax *et al.* (1976).



## Experimental

### Crystal data

$C_{31}H_{30}N_2O_2S$
$M_r$ = 494.63
Triclinic, $P\overline{1}$
$a$ = 10.9521 (3) Å
$b$ = 11.2563 (3) Å
$c$ = 12.5132 (3) Å
$\alpha$ = 100.930 (2)°
$\beta$ = 108.577 (1)°
$\gamma$ = 114.539 (1)°
$V$ = 1234.00 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.16 mm$^{-1}$
$T$ = 100 K
0.48 × 0.24 × 0.23 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.761, $T_{max}$ = 0.963
27773 measured reflections
6486 independent reflections
5001 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.112
$S$ = 1.01
6486 reflections
330 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.51 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| N2—H1*N*2$\cdots Cg2$ | 0.83 (2) | 2.61 (2) | 3.374 (2) | 152 (2) |
| C29—H29$\cdots Cg1^{i}$ | 0.93 | 2.90 | 3.605 (2) | 134 |

Symmetry code: (i) $x+1, y, z$. *Cg*1 and *Cg*2 are the centroids of the C19–C24 and C26–C31 rings, respectively.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2361).

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# supporting information

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

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

### S1. Comment

Pyrroloquinoline derivatives exhibit antitumor (Ferlin *et al.*, 2005; Dalla Via *et al.*, 2008), cytotoxic (Xiao *et al.*, 2006), antibacterial (Fujita *et al.*, 1996) and interferon-inducing activities (Crenshaw *et al.*, 1976). As part of our studies on pyrroloquinoline derivatives, we report here the crystal structure of the title compound.

In the title molecule, the pyrrolidine ring adopts a twist conformation; the asymmetry parameter $\Delta C_2$[C2—C10] (Duax *et al.*, 1976) and the puckering parameters $q_2$ and $\varphi$ (Cremer & Pople, 1975) are 7.5 (2)°, 0.394 (2) Å and 96.5 (3)°, respectively. The tosyl group is attached to the pyrrolidine ring in an equatorial position. The tetrahydropyridine ring adopts a half-chair conformation, with Q, $\theta$, $\varphi$ and $\Delta C_2$[C4—C9] values of 0.543 (2) Å, 131.1 (2)°, 93.1 (3)° and 6.6 (2)°, respectively. The phenyl group is attached to the tetrahydropyridine ring in a biaxial position. The C19—C24 phenyl ring forms dihedral angles of 74.0 (1) and 17.7 (1)°, respectively, with the C4—C9 and C12—C17 benzene rings. The C12—C17 and C26—C31 rings are oriented at a dihedral angle of 48.1 (1)°. The molecular structure is stabilized by an N—H···$\pi$ interaction (Table 1, Fig. 1). Bond lengths and angles are comparable to those observed in the 3-ethyl analogue (Sudha *et al.*, 2008).

In the crystal structure, molecules translated by one unit along the *a* axis are linked into chains by C—H···$\pi$ interactions (Fig.2, Table 1) involving the benzene ring of the tosyl group.

### S2. Experimental

$InCl_3$ (20 mol%) was added to a mixture of 2-(*N*-cinnamyl-*N*-tosylamino)-3-phenyl propanal (1 mmol) and aniline (1 mmol) in acetonitrile (20 ml). The reaction mixture was stirred at room temperature for 1 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 on silica gel 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) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$($C_{methyl}$). A rotating group model was used for the methyl groups.

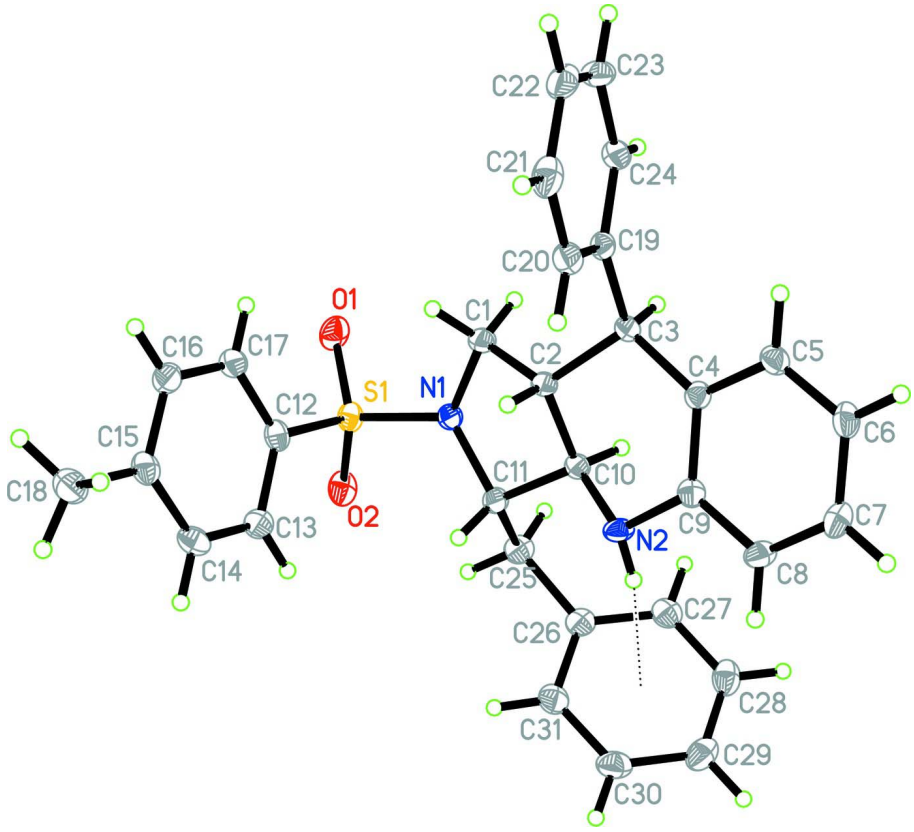


**Figure 1**

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radius. The dotted line indicates an N—H···$\pi$ interaction.

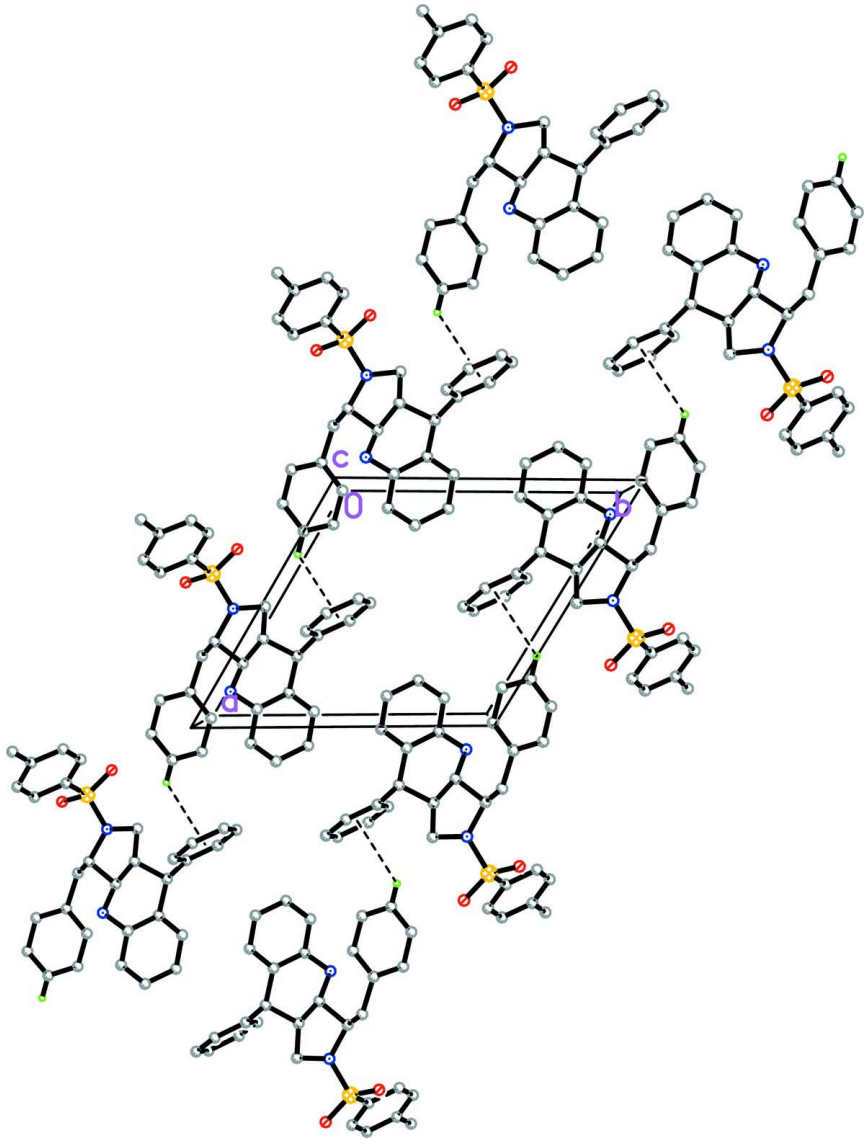


**Figure 2**

Crystal packing of the title compound. C—H···$\pi$ interactions are shown as dashed lines. For the sake of clarity, H atoms not involved in these interactions have been omitted.

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

*Crystal data*

$C_{31}H_{30}N_2O_2S$
$M_r = 494.63$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.9521$ (3) Å
$b = 11.2563$ (3) Å
$c = 12.5132$ (3) Å
$\alpha = 100.930$ (2)°
$\beta = 108.577$ (1)°
$\gamma = 114.539$ (1)°
$V = 1234.00$ (6) Å$^3$
$Z = 2$
$F(000) = 524$
$D_x = 1.331$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9232 reflections
$\theta = 2.3$–30.0°
$\mu = 0.16$ mm$^{-1}$

$T$ = 100 K
Block, colourless

0.48 × 0.24 × 0.23 mm

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.761, $T_{max}$ = 0.963

27773 measured reflections
6486 independent reflections
5001 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040
$\theta_{max}$ = 29.0°, $\theta_{min}$ = 2.1°
$h$ = −14→14
$k$ = −15→15
$l$ = −17→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.112
$S$ = 1.01
6486 reflections
330 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
$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 0.7475P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.51 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.36310 (4) | 0.70596 (4) | −0.01644 (4) | 0.01857 (10) |
| O1 | 0.25363 (13) | 0.74003 (13) | −0.07610 (11) | 0.0250 (3) |
| O2 | 0.40078 (13) | 0.62325 (12) | −0.08784 (10) | 0.0240 (3) |
| N1 | 0.51710 (14) | 0.85539 (13) | 0.07238 (12) | 0.0173 (3) |
| N2 | 0.87750 (15) | 1.02866 (14) | 0.33742 (12) | 0.0179 (3) |
| H1N2 | 0.939 (2) | 1.009 (2) | 0.3253 (18) | 0.026 (5)* |
| C1 | 0.50851 (17) | 0.96845 (16) | 0.14938 (14) | 0.0181 (3) |
| H1A | 0.4181 | 0.9292 | 0.1604 | 0.022* |
| H1B | 0.5109 | 1.0381 | 0.1136 | 0.022* |
| C2 | 0.64811 (17) | 1.03222 (15) | 0.26952 (14) | 0.0150 (3) |
| H2 | 0.6244 | 0.9770 | 0.3194 | 0.018* |
| C3 | 0.72246 (17) | 1.18825 (15) | 0.34620 (14) | 0.0151 (3) |
| H3 | 0.7343 | 1.2408 | 0.2925 | 0.018* |

| | | | | |
|---|---|---|---|---|
| C4 | 0.87963 (17) | 1.23749 (16) | 0.44241 (14) | 0.0158 (3) |
| C5 | 0.95793 (18) | 1.36418 (16) | 0.54193 (15) | 0.0185 (3) |
| H5 | 0.9122 | 1.4167 | 0.5496 | 0.022* |
| C6 | 1.10111 (18) | 1.41433 (17) | 0.62954 (15) | 0.0210 (3) |
| H6 | 1.1509 | 1.4995 | 0.6945 | 0.025* |
| C7 | 1.16958 (18) | 1.33567 (17) | 0.61916 (15) | 0.0215 (3) |
| H7 | 1.2659 | 1.3683 | 0.6774 | 0.026* |
| C8 | 1.09513 (18) | 1.20931 (17) | 0.52270 (15) | 0.0194 (3) |
| H8 | 1.1414 | 1.1570 | 0.5169 | 0.023* |
| C9 | 0.95044 (17) | 1.15885 (16) | 0.43336 (14) | 0.0165 (3) |
| C10 | 0.75726 (17) | 1.00918 (16) | 0.23056 (14) | 0.0156 (3) |
| H10 | 0.7982 | 1.0779 | 0.1954 | 0.019* |
| C11 | 0.66205 (17) | 0.86091 (16) | 0.13260 (14) | 0.0171 (3) |
| H11 | 0.6487 | 0.7906 | 0.1703 | 0.021* |
| C12 | 0.30055 (17) | 0.61554 (16) | 0.07342 (14) | 0.0183 (3) |
| C13 | 0.35945 (18) | 0.53371 (16) | 0.11236 (15) | 0.0207 (3) |
| H13 | 0.4332 | 0.5291 | 0.0933 | 0.025* |
| C14 | 0.30604 (19) | 0.45969 (17) | 0.17978 (15) | 0.0218 (3) |
| H14 | 0.3452 | 0.4057 | 0.2060 | 0.026* |
| C15 | 0.19503 (18) | 0.46425 (16) | 0.20920 (15) | 0.0202 (3) |
| C16 | 0.13799 (18) | 0.54575 (17) | 0.16856 (15) | 0.0217 (3) |
| H16 | 0.0632 | 0.5492 | 0.1866 | 0.026* |
| C17 | 0.19011 (18) | 0.62183 (16) | 0.10184 (15) | 0.0208 (3) |
| H17 | 0.1515 | 0.6765 | 0.0764 | 0.025* |
| C18 | 0.1399 (2) | 0.38679 (18) | 0.28517 (17) | 0.0254 (4) |
| H18A | 0.0355 | 0.3553 | 0.2593 | 0.038* |
| H18B | 0.1958 | 0.4487 | 0.3691 | 0.038* |
| H18C | 0.1533 | 0.3070 | 0.2755 | 0.038* |
| C19 | 0.63082 (17) | 1.21998 (16) | 0.40329 (14) | 0.0164 (3) |
| C20 | 0.61254 (18) | 1.17490 (17) | 0.49677 (15) | 0.0205 (3) |
| H20 | 0.6525 | 1.1206 | 0.5211 | 0.025* |
| C21 | 0.53582 (19) | 1.20987 (18) | 0.55365 (16) | 0.0254 (4) |
| H21 | 0.5250 | 1.1796 | 0.6160 | 0.031* |
| C22 | 0.47489 (19) | 1.29029 (18) | 0.51758 (17) | 0.0270 (4) |
| H22 | 0.4227 | 1.3134 | 0.5553 | 0.032* |
| C23 | 0.49216 (19) | 1.33563 (18) | 0.42575 (16) | 0.0248 (4) |
| H23 | 0.4523 | 1.3902 | 0.4021 | 0.030* |
| C24 | 0.56895 (18) | 1.30027 (16) | 0.36793 (15) | 0.0200 (3) |
| H24 | 0.5789 | 1.3305 | 0.3054 | 0.024* |
| C25 | 0.72722 (18) | 0.83906 (18) | 0.04379 (15) | 0.0213 (3) |
| H25A | 0.6672 | 0.7416 | −0.0120 | 0.026* |
| H25B | 0.7235 | 0.8977 | −0.0034 | 0.026* |
| C26 | 0.88731 (18) | 0.87601 (17) | 0.11140 (14) | 0.0193 (3) |
| C27 | 1.00564 (19) | 1.00373 (17) | 0.12935 (15) | 0.0219 (3) |
| H27 | 0.9855 | 1.0633 | 0.0942 | 0.026* |
| C28 | 1.1526 (2) | 1.04302 (18) | 0.19876 (16) | 0.0251 (4) |
| H28 | 1.2304 | 1.1272 | 0.2077 | 0.030* |
| C29 | 1.18447 (19) | 0.95779 (19) | 0.25491 (16) | 0.0262 (4) |

| | | | | |
|---|---|---|---|---|
| H29 | 1.2833 | 0.9853 | 0.3030 | 0.031* |
| C30 | 1.0679 (2) | 0.83100 (19) | 0.23886 (17) | 0.0259 (4) |
| H30 | 1.0886 | 0.7739 | 0.2773 | 0.031* |
| C31 | 0.92062 (19) | 0.78886 (17) | 0.16586 (16) | 0.0226 (4) |
| H31 | 0.8434 | 0.7019 | 0.1531 | 0.027* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.01624 (19) | 0.01639 (19) | 0.01461 (19) | 0.00506 (15) | 0.00412 (15) | 0.00178 (14) |
| O1 | 0.0177 (6) | 0.0274 (6) | 0.0207 (6) | 0.0083 (5) | 0.0026 (5) | 0.0090 (5) |
| O2 | 0.0232 (6) | 0.0204 (6) | 0.0171 (6) | 0.0060 (5) | 0.0082 (5) | −0.0016 (5) |
| N1 | 0.0150 (6) | 0.0137 (6) | 0.0176 (7) | 0.0066 (5) | 0.0048 (5) | 0.0009 (5) |
| N2 | 0.0174 (7) | 0.0189 (7) | 0.0163 (7) | 0.0124 (6) | 0.0047 (5) | 0.0017 (5) |
| C1 | 0.0167 (7) | 0.0165 (7) | 0.0197 (8) | 0.0095 (6) | 0.0072 (6) | 0.0033 (6) |
| C2 | 0.0156 (7) | 0.0141 (7) | 0.0158 (7) | 0.0083 (6) | 0.0074 (6) | 0.0043 (6) |
| C3 | 0.0156 (7) | 0.0134 (7) | 0.0160 (7) | 0.0076 (6) | 0.0070 (6) | 0.0042 (6) |
| C4 | 0.0149 (7) | 0.0154 (7) | 0.0166 (7) | 0.0069 (6) | 0.0077 (6) | 0.0053 (6) |
| C5 | 0.0200 (8) | 0.0152 (7) | 0.0207 (8) | 0.0091 (6) | 0.0106 (6) | 0.0046 (6) |
| C6 | 0.0179 (8) | 0.0163 (7) | 0.0188 (8) | 0.0042 (6) | 0.0062 (6) | 0.0012 (6) |
| C7 | 0.0146 (7) | 0.0235 (8) | 0.0186 (8) | 0.0064 (6) | 0.0052 (6) | 0.0042 (7) |
| C8 | 0.0178 (8) | 0.0227 (8) | 0.0206 (8) | 0.0129 (7) | 0.0088 (6) | 0.0074 (7) |
| C9 | 0.0172 (7) | 0.0164 (7) | 0.0158 (7) | 0.0081 (6) | 0.0085 (6) | 0.0048 (6) |
| C10 | 0.0157 (7) | 0.0144 (7) | 0.0154 (7) | 0.0078 (6) | 0.0064 (6) | 0.0035 (6) |
| C11 | 0.0153 (7) | 0.0154 (7) | 0.0164 (7) | 0.0074 (6) | 0.0049 (6) | 0.0022 (6) |
| C12 | 0.0179 (8) | 0.0135 (7) | 0.0148 (7) | 0.0045 (6) | 0.0047 (6) | 0.0011 (6) |
| C13 | 0.0203 (8) | 0.0175 (7) | 0.0209 (8) | 0.0094 (7) | 0.0091 (7) | 0.0016 (6) |
| C14 | 0.0270 (9) | 0.0176 (7) | 0.0226 (8) | 0.0135 (7) | 0.0112 (7) | 0.0055 (6) |
| C15 | 0.0212 (8) | 0.0136 (7) | 0.0184 (8) | 0.0059 (6) | 0.0071 (6) | 0.0013 (6) |
| C16 | 0.0182 (8) | 0.0198 (8) | 0.0246 (9) | 0.0089 (7) | 0.0097 (7) | 0.0052 (7) |
| C17 | 0.0182 (8) | 0.0163 (7) | 0.0229 (8) | 0.0082 (6) | 0.0063 (7) | 0.0042 (6) |
| C18 | 0.0301 (9) | 0.0217 (8) | 0.0292 (9) | 0.0142 (7) | 0.0165 (8) | 0.0109 (7) |
| C19 | 0.0138 (7) | 0.0133 (7) | 0.0163 (7) | 0.0050 (6) | 0.0056 (6) | 0.0012 (6) |
| C20 | 0.0201 (8) | 0.0176 (7) | 0.0220 (8) | 0.0088 (6) | 0.0096 (7) | 0.0058 (6) |
| C21 | 0.0212 (8) | 0.0238 (8) | 0.0224 (9) | 0.0050 (7) | 0.0119 (7) | 0.0029 (7) |
| C22 | 0.0177 (8) | 0.0249 (9) | 0.0282 (9) | 0.0077 (7) | 0.0109 (7) | −0.0037 (7) |
| C23 | 0.0201 (8) | 0.0224 (8) | 0.0289 (9) | 0.0138 (7) | 0.0081 (7) | 0.0016 (7) |
| C24 | 0.0185 (8) | 0.0165 (7) | 0.0203 (8) | 0.0086 (6) | 0.0062 (6) | 0.0030 (6) |
| C25 | 0.0215 (8) | 0.0218 (8) | 0.0173 (8) | 0.0116 (7) | 0.0073 (7) | 0.0018 (6) |
| C26 | 0.0212 (8) | 0.0201 (8) | 0.0157 (7) | 0.0120 (7) | 0.0090 (6) | 0.0002 (6) |
| C27 | 0.0253 (8) | 0.0210 (8) | 0.0200 (8) | 0.0126 (7) | 0.0113 (7) | 0.0053 (7) |
| C28 | 0.0229 (8) | 0.0221 (8) | 0.0231 (9) | 0.0070 (7) | 0.0118 (7) | 0.0024 (7) |
| C29 | 0.0191 (8) | 0.0304 (9) | 0.0229 (9) | 0.0123 (7) | 0.0075 (7) | 0.0019 (7) |
| C30 | 0.0296 (9) | 0.0260 (9) | 0.0277 (9) | 0.0198 (8) | 0.0124 (8) | 0.0082 (7) |
| C31 | 0.0243 (8) | 0.0183 (8) | 0.0245 (9) | 0.0114 (7) | 0.0124 (7) | 0.0030 (7) |

*Geometric parameters (Å, º)*

| | | | |
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| S1—O1 | 1.4360 (12) | C14—C15 | 1.395 (2) |
| S1—O2 | 1.4401 (12) | C14—H14 | 0.93 |
| S1—N1 | 1.6277 (13) | C15—C16 | 1.393 (2) |
| S1—C12 | 1.7649 (17) | C15—C18 | 1.507 (2) |
| N1—C11 | 1.4934 (19) | C16—C17 | 1.387 (2) |
| N1—C1 | 1.4996 (19) | C16—H16 | 0.93 |
| N2—C9 | 1.406 (2) | C17—H17 | 0.93 |
| N2—C10 | 1.448 (2) | C18—H18A | 0.96 |
| N2—H1N2 | 0.83 (2) | C18—H18B | 0.96 |
| C1—C2 | 1.526 (2) | C18—H18C | 0.96 |
| C1—H1A | 0.97 | C19—C24 | 1.393 (2) |
| C1—H1B | 0.97 | C19—C20 | 1.399 (2) |
| C2—C10 | 1.521 (2) | C20—C21 | 1.385 (2) |
| C2—C3 | 1.531 (2) | C20—H20 | 0.93 |
| C2—H2 | 0.98 | C21—C22 | 1.390 (3) |
| C3—C19 | 1.518 (2) | C21—H21 | 0.93 |
| C3—C4 | 1.534 (2) | C22—C23 | 1.377 (3) |
| C3—H3 | 0.98 | C22—H22 | 0.93 |
| C4—C5 | 1.397 (2) | C23—C24 | 1.395 (2) |
| C4—C9 | 1.409 (2) | C23—H23 | 0.93 |
| C5—C6 | 1.384 (2) | C24—H24 | 0.93 |
| C5—H5 | 0.93 | C25—C26 | 1.510 (2) |
| C6—C7 | 1.390 (2) | C25—H25A | 0.97 |
| C6—H6 | 0.93 | C25—H25B | 0.97 |
| C7—C8 | 1.380 (2) | C26—C27 | 1.393 (2) |
| C7—H7 | 0.93 | C26—C31 | 1.397 (2) |
| C8—C9 | 1.402 (2) | C27—C28 | 1.383 (2) |
| C8—H8 | 0.93 | C27—H27 | 0.93 |
| C10—C11 | 1.530 (2) | C28—C29 | 1.383 (3) |
| C10—H10 | 0.98 | C28—H28 | 0.93 |
| C11—C25 | 1.534 (2) | C29—C30 | 1.386 (3) |
| C11—H11 | 0.98 | C29—H29 | 0.93 |
| C12—C17 | 1.389 (2) | C30—C31 | 1.387 (2) |
| C12—C13 | 1.402 (2) | C30—H30 | 0.93 |
| C13—C14 | 1.387 (2) | C31—H31 | 0.93 |
| C13—H13 | 0.93 | | |

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|---|---|---|---|
| O1—S1—O2 | 119.68 (7) | C14—C13—C12 | 118.98 (15) |
| O1—S1—N1 | 106.27 (7) | C14—C13—H13 | 120.5 |
| O2—S1—N1 | 106.96 (7) | C12—C13—H13 | 120.5 |
| O1—S1—C12 | 107.58 (8) | C13—C14—C15 | 121.68 (15) |
| O2—S1—C12 | 107.09 (7) | C13—C14—H14 | 119.2 |
| N1—S1—C12 | 108.93 (7) | C15—C14—H14 | 119.2 |
| C11—N1—C1 | 111.99 (12) | C16—C15—C14 | 118.02 (16) |
| C11—N1—S1 | 120.85 (10) | C16—C15—C18 | 120.34 (15) |
| C1—N1—S1 | 118.57 (10) | C14—C15—C18 | 121.62 (15) |

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| C9—N2—C10 | 114.33 (12) | C17—C16—C15 | 121.59 (16) |
| C9—N2—H1N2 | 111.4 (14) | C17—C16—H16 | 119.2 |
| C10—N2—H1N2 | 116.0 (14) | C15—C16—H16 | 119.2 |
| N1—C1—C2 | 103.14 (12) | C16—C17—C12 | 119.40 (15) |
| N1—C1—H1A | 111.1 | C16—C17—H17 | 120.3 |
| C2—C1—H1A | 111.1 | C12—C17—H17 | 120.3 |
| N1—C1—H1B | 111.1 | C15—C18—H18A | 109.5 |
| C2—C1—H1B | 111.1 | C15—C18—H18B | 109.5 |
| H1A—C1—H1B | 109.1 | H18A—C18—H18B | 109.5 |
| C10—C2—C1 | 103.00 (12) | C15—C18—H18C | 109.5 |
| C10—C2—C3 | 109.13 (12) | H18A—C18—H18C | 109.5 |
| C1—C2—C3 | 118.14 (13) | H18B—C18—H18C | 109.5 |
| C10—C2—H2 | 108.7 | C24—C19—C20 | 118.41 (15) |
| C1—C2—H2 | 108.7 | C24—C19—C3 | 120.85 (14) |
| C3—C2—H2 | 108.7 | C20—C19—C3 | 120.67 (14) |
| C19—C3—C2 | 113.47 (12) | C21—C20—C19 | 120.97 (16) |
| C19—C3—C4 | 111.61 (12) | C21—C20—H20 | 119.5 |
| C2—C3—C4 | 108.54 (12) | C19—C20—H20 | 119.5 |
| C19—C3—H3 | 107.7 | C20—C21—C22 | 120.01 (17) |
| C2—C3—H3 | 107.7 | C20—C21—H21 | 120.0 |
| C4—C3—H3 | 107.7 | C22—C21—H21 | 120.0 |
| C5—C4—C9 | 117.86 (14) | C23—C22—C21 | 119.69 (16) |
| C5—C4—C3 | 120.29 (13) | C23—C22—H22 | 120.2 |
| C9—C4—C3 | 121.85 (13) | C21—C22—H22 | 120.2 |
| C6—C5—C4 | 122.35 (15) | C22—C23—C24 | 120.49 (16) |
| C6—C5—H5 | 118.8 | C22—C23—H23 | 119.8 |
| C4—C5—H5 | 118.8 | C24—C23—H23 | 119.8 |
| C5—C6—C7 | 119.10 (15) | C19—C24—C23 | 120.42 (16) |
| C5—C6—H6 | 120.4 | C19—C24—H24 | 119.8 |
| C7—C6—H6 | 120.4 | C23—C24—H24 | 119.8 |
| C8—C7—C6 | 120.19 (15) | C26—C25—C11 | 110.75 (13) |
| C8—C7—H7 | 119.9 | C26—C25—H25A | 109.5 |
| C6—C7—H7 | 119.9 | C11—C25—H25A | 109.5 |
| C7—C8—C9 | 120.77 (15) | C26—C25—H25B | 109.5 |
| C7—C8—H8 | 119.6 | C11—C25—H25B | 109.5 |
| C9—C8—H8 | 119.6 | H25A—C25—H25B | 108.1 |
| C8—C9—N2 | 119.04 (14) | C27—C26—C31 | 118.39 (15) |
| C8—C9—C4 | 119.73 (14) | C27—C26—C25 | 120.46 (15) |
| N2—C9—C4 | 121.22 (14) | C31—C26—C25 | 120.94 (15) |
| N2—C10—C2 | 107.97 (13) | C28—C27—C26 | 120.86 (16) |
| N2—C10—C11 | 115.04 (12) | C28—C27—H27 | 119.6 |
| C2—C10—C11 | 104.70 (12) | C26—C27—H27 | 119.6 |
| N2—C10—H10 | 109.6 | C27—C28—C29 | 120.38 (16) |
| C2—C10—H10 | 109.6 | C27—C28—H28 | 119.8 |
| C11—C10—H10 | 109.6 | C29—C28—H28 | 119.8 |
| N1—C11—C10 | 100.91 (11) | C28—C29—C30 | 119.44 (16) |
| N1—C11—C25 | 112.14 (13) | C28—C29—H29 | 120.3 |
| C10—C11—C25 | 113.02 (13) | C30—C29—H29 | 120.3 |

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|---|---|---|---|
| N1—C11—H11 | 110.2 | C29—C30—C31 | 120.37 (17) |
| C10—C11—H11 | 110.2 | C29—C30—H30 | 119.8 |
| C25—C11—H11 | 110.2 | C31—C30—H30 | 119.8 |
| C17—C12—C13 | 120.33 (15) | C30—C31—C26 | 120.50 (16) |
| C17—C12—S1 | 120.10 (13) | C30—C31—H31 | 119.8 |
| C13—C12—S1 | 119.54 (13) | C26—C31—H31 | 119.8 |
| | | | |
| O1—S1—N1—C11 | −169.30 (12) | N2—C10—C11—C25 | −86.66 (17) |
| O2—S1—N1—C11 | −40.37 (14) | C2—C10—C11—C25 | 155.01 (13) |
| C12—S1—N1—C11 | 75.06 (13) | O1—S1—C12—C17 | −16.92 (15) |
| O1—S1—N1—C1 | 45.43 (13) | O2—S1—C12—C17 | −146.77 (13) |
| O2—S1—N1—C1 | 174.35 (12) | N1—S1—C12—C17 | 97.88 (14) |
| C12—S1—N1—C1 | −70.22 (13) | O1—S1—C12—C13 | 160.95 (12) |
| C11—N1—C1—C2 | −7.78 (16) | O2—S1—C12—C13 | 31.10 (14) |
| S1—N1—C1—C2 | 140.39 (11) | N1—S1—C12—C13 | −84.25 (13) |
| N1—C1—C2—C10 | 29.34 (15) | C17—C12—C13—C14 | −0.2 (2) |
| N1—C1—C2—C3 | 149.66 (13) | S1—C12—C13—C14 | −178.03 (12) |
| C10—C2—C3—C19 | −172.66 (13) | C12—C13—C14—C15 | 0.3 (2) |
| C1—C2—C3—C19 | 70.25 (18) | C13—C14—C15—C16 | 0.1 (2) |
| C10—C2—C3—C4 | −47.97 (16) | C13—C14—C15—C18 | −178.40 (15) |
| C1—C2—C3—C4 | −165.07 (13) | C14—C15—C16—C17 | −0.7 (2) |
| C19—C3—C4—C5 | −38.87 (19) | C18—C15—C16—C17 | 177.88 (15) |
| C2—C3—C4—C5 | −164.65 (14) | C15—C16—C17—C12 | 0.8 (2) |
| C19—C3—C4—C9 | 141.90 (15) | C13—C12—C17—C16 | −0.4 (2) |
| C2—C3—C4—C9 | 16.12 (19) | S1—C12—C17—C16 | 177.50 (12) |
| C9—C4—C5—C6 | 0.7 (2) | C2—C3—C19—C24 | −113.47 (16) |
| C3—C4—C5—C6 | −178.57 (15) | C4—C3—C19—C24 | 123.52 (15) |
| C4—C5—C6—C7 | −0.5 (3) | C2—C3—C19—C20 | 69.60 (18) |
| C5—C6—C7—C8 | −0.1 (3) | C4—C3—C19—C20 | −53.42 (18) |
| C6—C7—C8—C9 | 0.6 (3) | C24—C19—C20—C21 | −0.5 (2) |
| C7—C8—C9—N2 | −179.10 (15) | C3—C19—C20—C21 | 176.54 (14) |
| C7—C8—C9—C4 | −0.4 (2) | C19—C20—C21—C22 | 0.4 (2) |
| C10—N2—C9—C8 | −159.03 (14) | C20—C21—C22—C23 | −0.4 (3) |
| C10—N2—C9—C4 | 22.3 (2) | C21—C22—C23—C24 | 0.6 (3) |
| C5—C4—C9—C8 | −0.2 (2) | C20—C19—C24—C23 | 0.7 (2) |
| C3—C4—C9—C8 | 179.05 (14) | C3—C19—C24—C23 | −176.33 (14) |
| C5—C4—C9—N2 | 178.46 (15) | C22—C23—C24—C19 | −0.8 (2) |
| C3—C4—C9—N2 | −2.3 (2) | N1—C11—C25—C26 | 167.76 (13) |
| C9—N2—C10—C2 | −55.04 (17) | C10—C11—C25—C26 | 54.52 (18) |
| C9—N2—C10—C11 | −171.53 (13) | C11—C25—C26—C27 | −102.25 (18) |
| C1—C2—C10—N2 | −164.09 (12) | C11—C25—C26—C31 | 72.43 (19) |
| C3—C2—C10—N2 | 69.58 (15) | C31—C26—C27—C28 | 0.4 (2) |
| C1—C2—C10—C11 | −41.05 (15) | C25—C26—C27—C28 | 175.20 (15) |
| C3—C2—C10—C11 | −167.38 (12) | C26—C27—C28—C29 | −2.0 (3) |
| C1—N1—C11—C10 | −16.78 (16) | C27—C28—C29—C30 | 1.4 (3) |
| S1—N1—C11—C10 | −164.12 (11) | C28—C29—C30—C31 | 0.9 (3) |
| C1—N1—C11—C25 | −137.32 (14) | C29—C30—C31—C26 | −2.5 (3) |
| S1—N1—C11—C25 | 75.33 (16) | C27—C26—C31—C30 | 1.9 (2) |

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| N2—C10—C11—N1 | 153.42 (13) | C25—C26—C31—C30 | −172.91 (15) |
| C2—C10—C11—N1 | 35.09 (15) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H1*N*2···*Cg*2 | 0.83 (2) | 2.61 (2) | 3.374 (2) | 152 (2) |
| C29—H29···*Cg*1$^{i}$ | 0.93 | 2.90 | 3.605 (2) | 134 |

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