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# 3-Benzyl-7-methoxy-9-phenyl-2-tosyl-2,3,3a,4,9,9a-hexahydro-1*H*-pyrrolo-[3,4-*b*]quinoline

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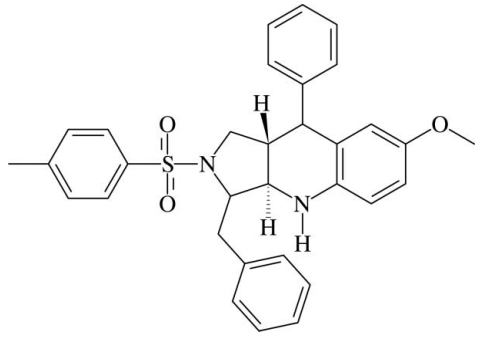
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.054; $wR$ factor = 0.155; data-to-parameter ratio = 17.4.

In the title compound, $C_{32}H_{32}N_2O_3S$, the pyrrolidine ring adopts an envelope conformation with the methine C atom nearest to the phenyl ring as the flap atom. The tetrahydropyridine ring has a half-chair conformation. The two rings are *trans*-fused. The phenyl ring bound to the tetrahydropyridine is oriented almost perpendicular [dihedral angle = 86.35 (10)°] to the fused benzene ring. The dihedral angle between the benzylphenyl ring and the sulfonyl-bound phenyl ring is 69.43 (10)°. A very weak N—H$\cdots\pi$ interaction is observed in the molecular structure. In the crystal, molecules translated one unit along the *b* axis are linked into *C*(10) chains by C—H$\cdots$O hydrogen bonds; adjacent chains are linked *via* C—H$\cdots\pi$ interactions, forming a two-dimensional network parallel to the *bc* plane.

## Related literature

For biological activity of pyrroloquinoline derivatives, see: Ryu *et al.* (2009); Tsuji *et al.* (1995); Ferlin *et al.* (2001). For related structures, see: Sudha *et al.* (2007, 2008*a*,*b*). For ring puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Duax *et al.* (1976).



## Experimental

### Crystal data

$C_{32}H_{32}N_2O_3S$
$M_r$ = 524.66
Monoclinic, $P2_1/c$
$a$ = 21.5063 (9) Å
$b$ = 11.6188 (5) Å
$c$ = 10.7616 (4) Å
$\beta$ = 98.219 (2)°
$V$ = 2661.46 (19) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.16 mm$^{-1}$
$T$ = 100 K
0.32 × 0.30 × 0.08 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.636, $T_{max}$ = 0.987
28181 measured reflections
6088 independent reflections
4661 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.155
$S$ = 1.02
6088 reflections
349 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.46 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.54 e Å$^{-3}$

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C30—H30$\cdots$O3$^{i}$ | 0.93 | 2.53 | 3.196 (3) | 128 |
| C24—H24$\cdots Cg1^{ii}$ | 0.93 | 2.56 | 3.476 (2) | 169 |
| N2—H1*N*2$\cdots Cg2$ | 0.88 (2) | 3.06 | 3.837 (2) | 147 |

Symmetry codes: (i) $x, y+1, z$; (ii) $x, -y-\frac{3}{2}, z-\frac{1}{2}$. *Cg*1 and *Cg*2 are the centroids of the C4–C9 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: LH2940).

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# supporting information

*Acta Cryst.* (2009). E**65**, o2956–o2957 [https://doi.org/10.1107/S1600536809044973]

## 3-Benzyl-7-methoxy-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 compounds exhibit antifungal (Ryu *et al.*, 2009), antibacterial (Tsuji *et al.*, 1995) and antiproliferative (Ferlin *et al.*, 2001) activities. We report here the crystal structure of the title compound, a pyrrolo[3,4-*b*]quinoline derivative.

The pyrrolidine ring adopts an envelope conformation with C2 as the flap atom. Atom C2 deviates by 0.663 (3) Å from the plane passing through the other four atoms of the ring (r.m.s. deviation 0.020 Å). The asymmetry parameter (Duax *et al.*, 1976) $\Delta C_s$[C2] = 5.4 (2)° and the puckering parameters (Cremer & Pople, 1975) $q_2$ = 0.439 (2) Å and $\varphi$ = 78.2 (3)°. The tosyl group is attached to the pyrrolidine ring in a biaxial position. The tetrahydropyridine ring adopts a half-chair conformation with an asymmetry parameter $\Delta C_2$[C2—C10] of 7.6 (2)°. The phenyl group attached to the tetrahydropyridine ring is also in a biaxial position. The dihedral angle between the C4—C9 and C19—C24 rings is 86.35 (10)° and that between the C12—C17 and C26—C31 rings is 69.43 (10)°. A very weak N—H···$\pi$ interaction (Table 1) is observed in the molecular structure. Bond lengths and angles are comparable with those observed in related structures (Sudha *et al.*, 2007,2008*a*,b).

In the crystal structure, molecules translated one unit along the *b* axis are linked into C(10) chains by C—H···O hydrogen bonds. Glide-related molecules in adjacent chains are linked *via* C—H···$\pi$ interactions involving the C4—C9 ring, forming a two-dimensional network parallel to the *bc* plane (Fig. 2).

### S2. Experimental

$InCl_3$ (20 mol%) was added to a mixture of 2-(*N*-cinnamyl-*N*-tosylamino)-3-phenyl propanal (1 mmol) and *p*-methoxy 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 in a difference map and refined freely [N—H = 0.88 (2) Å]. 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 methyl groups. Reflection 100 was partially obscured by the beam stop and was omitted.

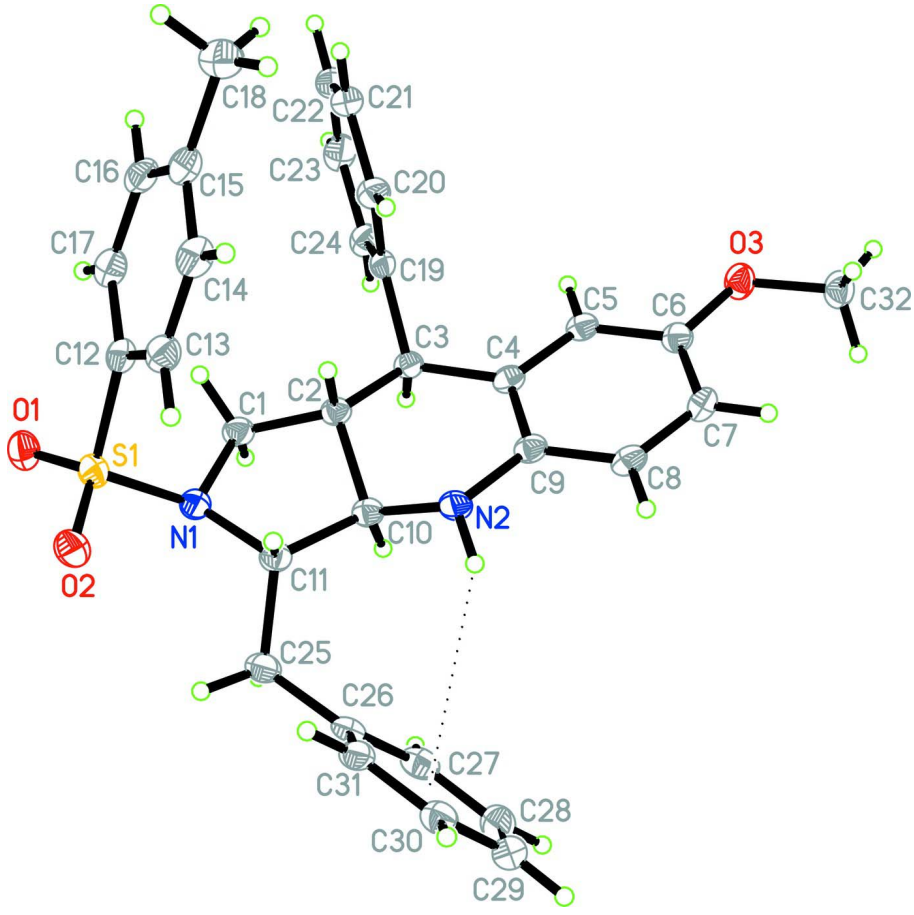


**Figure 1**

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

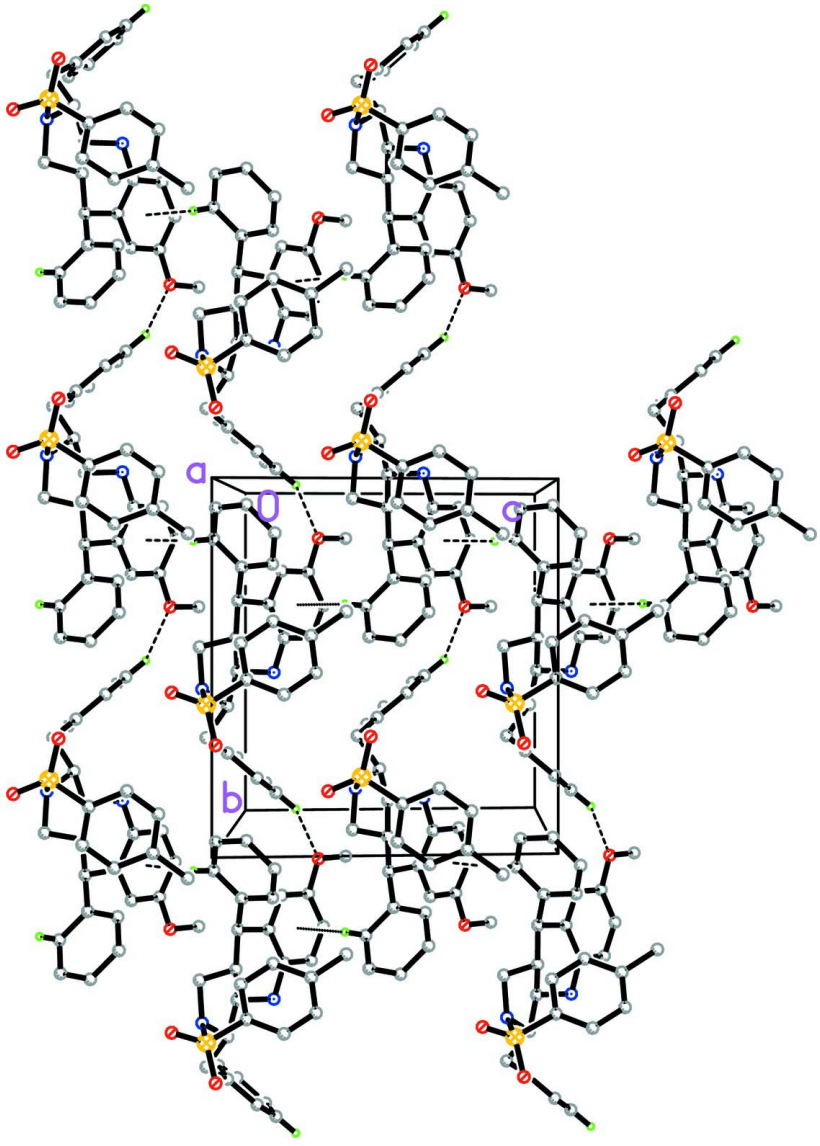


**Figure 2**

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

### 3-Benzyl-7-methoxy-9-phenyl-2-tosyl-2,3,3a,4,9,9a-hexahydro-1*H*- pyrrolo[3,4-*b*]quinoline

*Crystal data*

$C_{32}H_{32}N_2O_3S$
$M_r$ = 524.66
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 21.5063 (9) Å
$b$ = 11.6188 (5) Å
$c$ = 10.7616 (4) Å
$\beta$ = 98.219 (2)°
$V$ = 2661.46 (19) Å$^3$
$Z$ = 4
$F(000)$ = 1112
$D_x$ = 1.309 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 6305 reflections
$\theta$ = 2.6–28.5°
$\mu$ = 0.16 mm$^{-1}$
$T$ = 100 K
Plate, colourless
0.32 × 0.30 × 0.08 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)
$T_{min}$ = 0.636, $T_{max}$ = 0.987
28181 measured reflections
6088 independent reflections
4661 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.0°
$h$ = −23→27
$k$ = −15→14
$l$ = −13→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.155
$S$ = 1.02
6088 reflections
349 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
$w = 1/[\sigma^2(F_o^2) + (0.0891P)^2 + 0.9992P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.46 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.54 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.36811 (2) | 0.64135 (4) | −0.09053 (5) | 0.02080 (15) |
| O1 | 0.39510 (7) | 0.60291 (13) | −0.19725 (13) | 0.0264 (3) |
| O2 | 0.36734 (7) | 0.76149 (12) | −0.06064 (14) | 0.0266 (3) |
| O3 | 0.07988 (7) | 0.14332 (12) | 0.25445 (14) | 0.0235 (3) |
| N1 | 0.29441 (8) | 0.59952 (14) | −0.11262 (15) | 0.0197 (4) |
| N2 | 0.18416 (8) | 0.55576 (14) | 0.11176 (16) | 0.0202 (4) |
| H1N2 | 0.1626 (11) | 0.619 (2) | 0.122 (2) | 0.024 (6)* |
| C1 | 0.28306 (10) | 0.47333 (16) | −0.12239 (18) | 0.0195 (4) |
| H1A | 0.3222 | 0.4312 | −0.1194 | 0.023* |
| H1B | 0.2557 | 0.4539 | −0.1991 | 0.023* |
| C2 | 0.25163 (9) | 0.44865 (15) | −0.00752 (17) | 0.0172 (4) |
| H2 | 0.2834 | 0.4530 | 0.0673 | 0.021* |
| C3 | 0.21612 (9) | 0.33569 (15) | −0.00428 (17) | 0.0169 (4) |
| H3 | 0.1899 | 0.3268 | −0.0860 | 0.020* |
| C4 | 0.17183 (9) | 0.34490 (16) | 0.09480 (17) | 0.0176 (4) |

| | | | | |
|---|---|---|---|---|
| C5 | 0.14457 (9) | 0.24516 (16) | 0.13452 (18) | 0.0182 (4) |
| H5 | 0.1546 | 0.1747 | 0.1016 | 0.022* |
| C6 | 0.10267 (9) | 0.24795 (16) | 0.22227 (18) | 0.0194 (4) |
| C7 | 0.08772 (10) | 0.35345 (17) | 0.27171 (19) | 0.0213 (4) |
| H7 | 0.0602 | 0.3569 | 0.3308 | 0.026* |
| C8 | 0.11424 (10) | 0.45329 (17) | 0.23202 (19) | 0.0213 (4) |
| H8 | 0.1037 | 0.5236 | 0.2648 | 0.026* |
| C9 | 0.15627 (9) | 0.45154 (16) | 0.14423 (18) | 0.0181 (4) |
| C10 | 0.20811 (9) | 0.55138 (16) | −0.00791 (18) | 0.0179 (4) |
| H10 | 0.1731 | 0.5435 | −0.0764 | 0.022* |
| C11 | 0.24967 (10) | 0.65334 (16) | −0.03459 (18) | 0.0192 (4) |
| H11 | 0.2727 | 0.6828 | 0.0441 | 0.023* |
| C12 | 0.40517 (9) | 0.56541 (17) | 0.04217 (18) | 0.0206 (4) |
| C13 | 0.40440 (10) | 0.60984 (18) | 0.16170 (19) | 0.0231 (4) |
| H13 | 0.3878 | 0.6825 | 0.1723 | 0.028* |
| C14 | 0.42880 (10) | 0.54439 (18) | 0.2653 (2) | 0.0249 (5) |
| H14 | 0.4288 | 0.5744 | 0.3454 | 0.030* |
| C15 | 0.45327 (10) | 0.43488 (19) | 0.2518 (2) | 0.0251 (5) |
| C16 | 0.45382 (10) | 0.39268 (18) | 0.1305 (2) | 0.0238 (4) |
| H16 | 0.4702 | 0.3199 | 0.1197 | 0.029* |
| C17 | 0.43044 (10) | 0.45702 (17) | 0.0261 (2) | 0.0233 (4) |
| H17 | 0.4316 | 0.4281 | −0.0541 | 0.028* |
| C18 | 0.47876 (12) | 0.3636 (2) | 0.3642 (2) | 0.0334 (5) |
| H18A | 0.4656 | 0.3963 | 0.4382 | 0.050* |
| H18B | 0.5238 | 0.3627 | 0.3732 | 0.050* |
| H18C | 0.4631 | 0.2864 | 0.3531 | 0.050* |
| C19 | 0.26098 (9) | 0.23397 (16) | 0.01226 (18) | 0.0177 (4) |
| C20 | 0.30745 (10) | 0.22449 (17) | 0.11657 (19) | 0.0220 (4) |
| H20 | 0.3105 | 0.2803 | 0.1791 | 0.026* |
| C21 | 0.34910 (10) | 0.13259 (18) | 0.1278 (2) | 0.0254 (5) |
| H21 | 0.3800 | 0.1277 | 0.1974 | 0.030* |
| C22 | 0.34495 (11) | 0.04784 (17) | 0.0358 (2) | 0.0268 (5) |
| H22 | 0.3725 | −0.0143 | 0.0441 | 0.032* |
| C23 | 0.29953 (11) | 0.05698 (17) | −0.0680 (2) | 0.0269 (5) |
| H23 | 0.2968 | 0.0013 | −0.1306 | 0.032* |
| C24 | 0.25761 (10) | 0.14916 (17) | −0.0797 (2) | 0.0223 (4) |
| H24 | 0.2270 | 0.1540 | −0.1499 | 0.027* |
| C25 | 0.21481 (10) | 0.75164 (17) | −0.10939 (19) | 0.0227 (4) |
| H25A | 0.2447 | 0.8112 | −0.1230 | 0.027* |
| H25B | 0.1962 | 0.7229 | −0.1909 | 0.027* |
| C26 | 0.16400 (10) | 0.80340 (16) | −0.04408 (18) | 0.0202 (4) |
| C27 | 0.10099 (10) | 0.77711 (17) | −0.0814 (2) | 0.0249 (5) |
| H27 | 0.0900 | 0.7246 | −0.1461 | 0.030* |
| C28 | 0.05413 (11) | 0.82820 (19) | −0.0235 (2) | 0.0276 (5) |
| H28 | 0.0122 | 0.8108 | −0.0503 | 0.033* |
| C29 | 0.07005 (11) | 0.90497 (18) | 0.0741 (2) | 0.0275 (5) |
| H29 | 0.0388 | 0.9400 | 0.1124 | 0.033* |
| C30 | 0.13279 (10) | 0.92955 (17) | 0.1147 (2) | 0.0237 (4) |

| | | | | |
|---|---|---|---|---|
| H30 | 0.1437 | 0.9797 | 0.1817 | 0.028* |
| C31 | 0.17939 (10) | 0.87961 (16) | 0.05583 (19) | 0.0213 (4) |
| H31 | 0.2213 | 0.8971 | 0.0832 | 0.026* |
| C32 | 0.03712 (10) | 0.14275 (18) | 0.3447 (2) | 0.0255 (5) |
| H32A | 0.0236 | 0.0653 | 0.3568 | 0.038* |
| H32B | 0.0014 | 0.1897 | 0.3150 | 0.038* |
| H32C | 0.0577 | 0.1728 | 0.4230 | 0.038* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0206 (3) | 0.0180 (3) | 0.0242 (3) | −0.00236 (19) | 0.0046 (2) | 0.00132 (18) |
| O1 | 0.0265 (9) | 0.0282 (8) | 0.0259 (8) | −0.0026 (6) | 0.0091 (6) | 0.0015 (6) |
| O2 | 0.0252 (9) | 0.0192 (7) | 0.0353 (8) | −0.0044 (6) | 0.0042 (7) | 0.0022 (6) |
| O3 | 0.0211 (8) | 0.0197 (7) | 0.0313 (8) | −0.0037 (6) | 0.0089 (6) | −0.0016 (6) |
| N1 | 0.0190 (9) | 0.0161 (8) | 0.0245 (9) | 0.0001 (7) | 0.0044 (7) | 0.0006 (6) |
| N2 | 0.0250 (10) | 0.0124 (8) | 0.0243 (9) | 0.0029 (7) | 0.0075 (7) | −0.0008 (6) |
| C1 | 0.0199 (11) | 0.0162 (9) | 0.0222 (10) | 0.0009 (7) | 0.0029 (8) | −0.0006 (7) |
| C2 | 0.0164 (10) | 0.0145 (9) | 0.0204 (9) | 0.0006 (7) | 0.0014 (8) | −0.0007 (7) |
| C3 | 0.0156 (10) | 0.0159 (9) | 0.0189 (9) | 0.0004 (7) | 0.0015 (7) | −0.0002 (7) |
| C4 | 0.0150 (10) | 0.0182 (9) | 0.0188 (9) | 0.0020 (7) | −0.0007 (7) | −0.0015 (7) |
| C5 | 0.0161 (10) | 0.0155 (9) | 0.0223 (10) | 0.0012 (7) | 0.0008 (8) | −0.0015 (7) |
| C6 | 0.0154 (10) | 0.0179 (9) | 0.0242 (10) | −0.0018 (7) | 0.0007 (8) | 0.0005 (7) |
| C7 | 0.0158 (10) | 0.0246 (10) | 0.0245 (10) | 0.0012 (8) | 0.0056 (8) | −0.0012 (8) |
| C8 | 0.0189 (11) | 0.0180 (10) | 0.0270 (10) | 0.0039 (8) | 0.0030 (8) | −0.0035 (8) |
| C9 | 0.0144 (10) | 0.0169 (9) | 0.0222 (10) | 0.0002 (7) | −0.0009 (8) | −0.0010 (7) |
| C10 | 0.0182 (10) | 0.0163 (9) | 0.0190 (9) | 0.0006 (7) | 0.0017 (8) | −0.0003 (7) |
| C11 | 0.0196 (11) | 0.0159 (9) | 0.0224 (10) | 0.0010 (7) | 0.0038 (8) | −0.0009 (7) |
| C12 | 0.0152 (10) | 0.0221 (10) | 0.0248 (10) | −0.0020 (8) | 0.0038 (8) | 0.0008 (8) |
| C13 | 0.0208 (11) | 0.0205 (10) | 0.0282 (11) | −0.0011 (8) | 0.0045 (8) | −0.0022 (8) |
| C14 | 0.0212 (11) | 0.0296 (11) | 0.0239 (10) | −0.0007 (9) | 0.0035 (8) | −0.0036 (8) |
| C15 | 0.0151 (11) | 0.0296 (11) | 0.0301 (11) | −0.0011 (8) | 0.0022 (8) | 0.0031 (9) |
| C16 | 0.0151 (10) | 0.0226 (10) | 0.0336 (11) | 0.0003 (8) | 0.0035 (8) | −0.0014 (8) |
| C17 | 0.0205 (11) | 0.0236 (10) | 0.0266 (11) | −0.0016 (8) | 0.0058 (8) | −0.0043 (8) |
| C18 | 0.0320 (14) | 0.0355 (13) | 0.0325 (12) | 0.0057 (10) | 0.0036 (10) | 0.0063 (10) |
| C19 | 0.0160 (10) | 0.0147 (9) | 0.0235 (10) | −0.0002 (7) | 0.0068 (8) | 0.0028 (7) |
| C20 | 0.0225 (11) | 0.0212 (10) | 0.0228 (10) | 0.0027 (8) | 0.0046 (8) | 0.0006 (8) |
| C21 | 0.0212 (11) | 0.0280 (11) | 0.0277 (11) | 0.0056 (9) | 0.0058 (9) | 0.0086 (8) |
| C22 | 0.0267 (12) | 0.0169 (10) | 0.0399 (12) | 0.0061 (8) | 0.0152 (10) | 0.0061 (8) |
| C23 | 0.0274 (12) | 0.0169 (10) | 0.0386 (12) | −0.0010 (8) | 0.0127 (10) | −0.0058 (9) |
| C24 | 0.0199 (11) | 0.0197 (10) | 0.0277 (11) | −0.0021 (8) | 0.0047 (8) | −0.0026 (8) |
| C25 | 0.0269 (12) | 0.0178 (10) | 0.0237 (10) | 0.0034 (8) | 0.0044 (9) | 0.0038 (8) |
| C26 | 0.0241 (11) | 0.0126 (9) | 0.0238 (10) | 0.0023 (7) | 0.0032 (8) | 0.0059 (7) |
| C27 | 0.0287 (12) | 0.0176 (9) | 0.0271 (11) | −0.0024 (8) | −0.0006 (9) | 0.0027 (8) |
| C28 | 0.0189 (11) | 0.0301 (11) | 0.0331 (12) | −0.0022 (9) | 0.0011 (9) | 0.0079 (9) |
| C29 | 0.0248 (12) | 0.0253 (11) | 0.0342 (12) | 0.0049 (9) | 0.0099 (9) | 0.0075 (9) |
| C30 | 0.0280 (12) | 0.0173 (9) | 0.0264 (10) | 0.0005 (8) | 0.0057 (9) | 0.0021 (8) |
| C31 | 0.0193 (11) | 0.0158 (9) | 0.0282 (11) | 0.0005 (8) | 0.0015 (8) | 0.0038 (8) |

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|---|---|---|---|---|---|---|
| C32 | 0.0210 (11) | 0.0261 (11) | 0.0307 (11) | −0.0041 (8) | 0.0080 (9) | 0.0006 (9) |

*Geometric parameters (Å, º)*

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| S1—O1 | 1.4303 (15) | C14—H14 | 0.93 |
| S1—O2 | 1.4332 (15) | C15—C16 | 1.396 (3) |
| S1—N1 | 1.6424 (18) | C15—C18 | 1.504 (3) |
| S1—C12 | 1.768 (2) | C16—C17 | 1.383 (3) |
| O3—C6 | 1.374 (2) | C16—H16 | 0.93 |
| O3—C32 | 1.430 (2) | C17—H17 | 0.93 |
| N1—C1 | 1.488 (2) | C18—H18A | 0.96 |
| N1—C11 | 1.501 (2) | C18—H18B | 0.96 |
| N2—C9 | 1.417 (2) | C18—H18C | 0.96 |
| N2—C10 | 1.455 (2) | C19—C24 | 1.391 (3) |
| N2—H1N2 | 0.88 (2) | C19—C20 | 1.396 (3) |
| C1—C2 | 1.519 (3) | C20—C21 | 1.388 (3) |
| C1—H1A | 0.97 | C20—H20 | 0.93 |
| C1—H1B | 0.97 | C21—C22 | 1.390 (3) |
| C2—C10 | 1.516 (3) | C21—H21 | 0.93 |
| C2—C3 | 1.521 (3) | C22—C23 | 1.379 (3) |
| C2—H2 | 0.98 | C22—H22 | 0.93 |
| C3—C19 | 1.520 (3) | C23—C24 | 1.394 (3) |
| C3—C4 | 1.532 (3) | C23—H23 | 0.93 |
| C3—H3 | 0.98 | C24—H24 | 0.93 |
| C4—C5 | 1.393 (3) | C25—C26 | 1.506 (3) |
| C4—C9 | 1.407 (3) | C25—H25A | 0.97 |
| C5—C6 | 1.396 (3) | C25—H25B | 0.97 |
| C5—H5 | 0.93 | C26—C27 | 1.391 (3) |
| C6—C7 | 1.392 (3) | C26—C31 | 1.396 (3) |
| C7—C8 | 1.387 (3) | C27—C28 | 1.392 (3) |
| C7—H7 | 0.93 | C27—H27 | 0.93 |
| C8—C9 | 1.398 (3) | C28—C29 | 1.383 (3) |
| C8—H8 | 0.93 | C28—H28 | 0.93 |
| C10—C11 | 1.536 (3) | C29—C30 | 1.387 (3) |
| C10—H10 | 0.98 | C29—H29 | 0.93 |
| C11—C25 | 1.530 (3) | C30—C31 | 1.387 (3) |
| C11—H11 | 0.98 | C30—H30 | 0.93 |
| C12—C13 | 1.388 (3) | C31—H31 | 0.93 |
| C12—C17 | 1.392 (3) | C32—H32A | 0.96 |
| C13—C14 | 1.389 (3) | C32—H32B | 0.96 |
| C13—H13 | 0.93 | C32—H32C | 0.96 |
| C14—C15 | 1.392 (3) | | |

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| O1—S1—O2 | 120.22 (9) | C13—C14—C15 | 121.46 (19) |
| O1—S1—N1 | 106.58 (9) | C13—C14—H14 | 119.3 |
| O2—S1—N1 | 106.18 (9) | C15—C14—H14 | 119.3 |
| O1—S1—C12 | 107.76 (9) | C14—C15—C16 | 118.19 (19) |
| O2—S1—C12 | 108.85 (9) | C14—C15—C18 | 121.25 (19) |

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| N1—S1—C12 | 106.47 (9) | C16—C15—C18 | 120.6 (2) |
| C6—O3—C32 | 117.56 (15) | C17—C16—C15 | 121.27 (19) |
| C1—N1—C11 | 109.76 (15) | C17—C16—H16 | 119.4 |
| C1—N1—S1 | 116.56 (13) | C15—C16—H16 | 119.4 |
| C11—N1—S1 | 118.58 (13) | C16—C17—C12 | 119.42 (19) |
| C9—N2—C10 | 113.85 (15) | C16—C17—H17 | 120.3 |
| C9—N2—H1N2 | 115.6 (15) | C12—C17—H17 | 120.3 |
| C10—N2—H1N2 | 113.5 (15) | C15—C18—H18A | 109.5 |
| N1—C1—C2 | 102.50 (15) | C15—C18—H18B | 109.5 |
| N1—C1—H1A | 111.3 | H18A—C18—H18B | 109.5 |
| C2—C1—H1A | 111.3 | C15—C18—H18C | 109.5 |
| N1—C1—H1B | 111.3 | H18A—C18—H18C | 109.5 |
| C2—C1—H1B | 111.3 | H18B—C18—H18C | 109.5 |
| H1A—C1—H1B | 109.2 | C24—C19—C20 | 118.32 (18) |
| C10—C2—C1 | 101.27 (15) | C24—C19—C3 | 120.00 (18) |
| C10—C2—C3 | 111.56 (16) | C20—C19—C3 | 121.65 (17) |
| C1—C2—C3 | 117.70 (15) | C21—C20—C19 | 120.63 (19) |
| C10—C2—H2 | 108.6 | C21—C20—H20 | 119.7 |
| C1—C2—H2 | 108.6 | C19—C20—H20 | 119.7 |
| C3—C2—H2 | 108.6 | C20—C21—C22 | 120.5 (2) |
| C19—C3—C2 | 111.18 (16) | C20—C21—H21 | 119.7 |
| C19—C3—C4 | 114.85 (15) | C22—C21—H21 | 119.7 |
| C2—C3—C4 | 108.65 (15) | C23—C22—C21 | 119.24 (19) |
| C19—C3—H3 | 107.3 | C23—C22—H22 | 120.4 |
| C2—C3—H3 | 107.3 | C21—C22—H22 | 120.4 |
| C4—C3—H3 | 107.3 | C22—C23—C24 | 120.41 (19) |
| C5—C4—C9 | 118.88 (18) | C22—C23—H23 | 119.8 |
| C5—C4—C3 | 119.10 (16) | C24—C23—H23 | 119.8 |
| C9—C4—C3 | 121.99 (17) | C19—C24—C23 | 120.9 (2) |
| C4—C5—C6 | 121.94 (17) | C19—C24—H24 | 119.6 |
| C4—C5—H5 | 119.0 | C23—C24—H24 | 119.6 |
| C6—C5—H5 | 119.0 | C26—C25—C11 | 112.71 (16) |
| O3—C6—C7 | 124.94 (18) | C26—C25—H25A | 109.1 |
| O3—C6—C5 | 115.99 (17) | C11—C25—H25A | 109.1 |
| C7—C6—C5 | 119.07 (18) | C26—C25—H25B | 109.1 |
| C8—C7—C6 | 119.42 (18) | C11—C25—H25B | 109.1 |
| C8—C7—H7 | 120.3 | H25A—C25—H25B | 107.8 |
| C6—C7—H7 | 120.3 | C27—C26—C31 | 118.40 (19) |
| C7—C8—C9 | 122.02 (18) | C27—C26—C25 | 121.28 (19) |
| C7—C8—H8 | 119.0 | C31—C26—C25 | 120.32 (19) |
| C9—C8—H8 | 119.0 | C26—C27—C28 | 121.0 (2) |
| C8—C9—C4 | 118.68 (17) | C26—C27—H27 | 119.5 |
| C8—C9—N2 | 119.44 (17) | C28—C27—H27 | 119.5 |
| C4—C9—N2 | 121.81 (17) | C29—C28—C27 | 119.9 (2) |
| N2—C10—C2 | 108.76 (15) | C29—C28—H28 | 120.0 |
| N2—C10—C11 | 115.32 (16) | C27—C28—H28 | 120.0 |
| C2—C10—C11 | 103.43 (16) | C28—C29—C30 | 119.7 (2) |
| N2—C10—H10 | 109.7 | C28—C29—H29 | 120.1 |

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| C2—C10—H10 | 109.7 | C30—C29—H29 | 120.1 |
| C11—C10—H10 | 109.7 | C31—C30—C29 | 120.2 (2) |
| N1—C11—C25 | 108.76 (15) | C31—C30—H30 | 119.9 |
| N1—C11—C10 | 102.71 (14) | C29—C30—H30 | 119.9 |
| C25—C11—C10 | 114.82 (17) | C30—C31—C26 | 120.7 (2) |
| N1—C11—H11 | 110.1 | C30—C31—H31 | 119.7 |
| C25—C11—H11 | 110.1 | C26—C31—H31 | 119.7 |
| C10—C11—H11 | 110.1 | O3—C32—H32A | 109.5 |
| C13—C12—C17 | 120.53 (19) | O3—C32—H32B | 109.5 |
| C13—C12—S1 | 119.93 (16) | H32A—C32—H32B | 109.5 |
| C17—C12—S1 | 119.33 (15) | O3—C32—H32C | 109.5 |
| C12—C13—C14 | 119.12 (19) | H32A—C32—H32C | 109.5 |
| C12—C13—H13 | 120.4 | H32B—C32—H32C | 109.5 |
| C14—C13—H13 | 120.4 | | |

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| O1—S1—N1—C1 | 61.38 (15) | N2—C10—C11—N1 | 148.55 (16) |
| O2—S1—N1—C1 | −169.33 (13) | C2—C10—C11—N1 | 29.94 (19) |
| C12—S1—N1—C1 | −53.44 (16) | N2—C10—C11—C25 | −93.6 (2) |
| O1—S1—N1—C11 | −163.96 (13) | C2—C10—C11—C25 | 147.81 (16) |
| O2—S1—N1—C11 | −34.67 (16) | O1—S1—C12—C13 | 158.49 (16) |
| C12—S1—N1—C11 | 81.22 (15) | O2—S1—C12—C13 | 26.59 (19) |
| C11—N1—C1—C2 | −23.1 (2) | N1—S1—C12—C13 | −87.49 (18) |
| S1—N1—C1—C2 | 115.35 (15) | O1—S1—C12—C17 | −26.68 (19) |
| N1—C1—C2—C10 | 40.98 (18) | O2—S1—C12—C17 | −158.58 (16) |
| N1—C1—C2—C3 | 162.85 (16) | N1—S1—C12—C17 | 87.34 (18) |
| C10—C2—C3—C19 | −173.02 (15) | C17—C12—C13—C14 | −0.4 (3) |
| C1—C2—C3—C19 | 70.6 (2) | S1—C12—C13—C14 | 174.34 (16) |
| C10—C2—C3—C4 | −45.7 (2) | C12—C13—C14—C15 | −0.8 (3) |
| C1—C2—C3—C4 | −162.10 (16) | C13—C14—C15—C16 | 1.2 (3) |
| C19—C3—C4—C5 | −40.9 (2) | C13—C14—C15—C18 | −179.1 (2) |
| C2—C3—C4—C5 | −166.12 (17) | C14—C15—C16—C17 | −0.4 (3) |
| C19—C3—C4—C9 | 141.09 (18) | C18—C15—C16—C17 | 179.9 (2) |
| C2—C3—C4—C9 | 15.9 (2) | C15—C16—C17—C12 | −0.8 (3) |
| C9—C4—C5—C6 | −0.4 (3) | C13—C12—C17—C16 | 1.2 (3) |
| C3—C4—C5—C6 | −178.46 (18) | S1—C12—C17—C16 | −173.61 (16) |
| C32—O3—C6—C7 | 0.6 (3) | C2—C3—C19—C24 | −118.83 (19) |
| C32—O3—C6—C5 | 179.61 (18) | C4—C3—C19—C24 | 117.29 (19) |
| C4—C5—C6—O3 | −179.17 (17) | C2—C3—C19—C20 | 59.2 (2) |
| C4—C5—C6—C7 | −0.1 (3) | C4—C3—C19—C20 | −64.7 (2) |
| O3—C6—C7—C8 | 179.58 (19) | C24—C19—C20—C21 | 0.0 (3) |
| C5—C6—C7—C8 | 0.6 (3) | C3—C19—C20—C21 | −178.04 (18) |
| C6—C7—C8—C9 | −0.6 (3) | C19—C20—C21—C22 | −0.5 (3) |
| C7—C8—C9—C4 | 0.1 (3) | C20—C21—C22—C23 | 1.0 (3) |
| C7—C8—C9—N2 | −177.01 (19) | C21—C22—C23—C24 | −1.0 (3) |
| C5—C4—C9—C8 | 0.4 (3) | C20—C19—C24—C23 | 0.0 (3) |
| C3—C4—C9—C8 | 178.37 (17) | C3—C19—C24—C23 | 178.09 (18) |
| C5—C4—C9—N2 | 177.43 (18) | C22—C23—C24—C19 | 0.5 (3) |
| C3—C4—C9—N2 | −4.6 (3) | N1—C11—C25—C26 | 174.16 (16) |

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| C10—N2—C9—C8 | −159.30 (18) | C10—C11—C25—C26 | 59.8 (2) |
| C10—N2—C9—C4 | 23.6 (3) | C11—C25—C26—C27 | −102.6 (2) |
| C9—N2—C10—C2 | −53.1 (2) | C11—C25—C26—C31 | 77.6 (2) |
| C9—N2—C10—C11 | −168.66 (16) | C31—C26—C27—C28 | 2.0 (3) |
| C1—C2—C10—N2 | −167.42 (15) | C25—C26—C27—C28 | −177.81 (18) |
| C3—C2—C10—N2 | 66.5 (2) | C26—C27—C28—C29 | −1.1 (3) |
| C1—C2—C10—C11 | −44.36 (18) | C27—C28—C29—C30 | −0.8 (3) |
| C3—C2—C10—C11 | −170.41 (15) | C28—C29—C30—C31 | 1.6 (3) |
| C1—N1—C11—C25 | −126.22 (17) | C29—C30—C31—C26 | −0.5 (3) |
| S1—N1—C11—C25 | 96.32 (18) | C27—C26—C31—C30 | −1.2 (3) |
| C1—N1—C11—C10 | −4.1 (2) | C25—C26—C31—C30 | 178.62 (18) |
| S1—N1—C11—C10 | −141.61 (14) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C30—H30···O3$^{i}$ | 0.93 | 2.53 | 3.196 (3) | 128 |
| C24—H24···*Cg*1$^{ii}$ | 0.93 | 2.56 | 3.476 (2) | 169 |
| N2—H1*N*2···*Cg*2 | 0.88 (2) | 3.06 | 3.837 (2) | 147 |

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*, −*y*−3/2, *z*−1/2.