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# 4-Benzyl-2-(4-chlorobenzylidene)-3,4-dihydro-2*H*-1,4-benzothiazin-3(4*H*)-one

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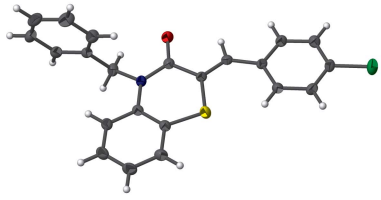
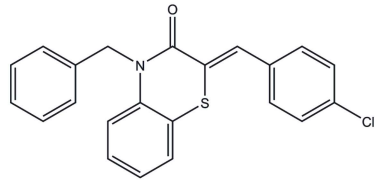
**Structural data**: full structural data are available from iucrdata.iucr.org

The title compound, $C_{22}H_{16}ClNOS$, has three aromatic systems, *viz*. (i) a phenyl ring, (ii) a chlorobenzene ring and (iii) a 1,4-benzothiazine fused-ring system (r.m.s. deviation of the ten fitted atoms = 0.023 Å). The dihedral angle between planes (ii) and (iii) is 1.68 (8)°, indicating a coplanar arrangement, and between plane (i) and each of (ii) and (iii) is 85.61 (8) and 86.74 (8)°, respectively, indicating the phenyl ring is approximately perpendicular to the remaining residue. In the crystal, pairwise methylene-C—H···O(carbonyl) hydrogen bonds form dimers which stack along the *b*-axis direction.

**3D view**



**Chemical scheme**




## Structure description

Several sulfur- and nitrogen-containing heterocyclic compounds have been well studied. Various 1,4-benzothiazine derivatives have been synthesized by several methods (Parai & Panda, 2009; Barange *et al.*, 2007; Saadouni *et al.*, 2014). 1,4-Benzothiazine derivatives are important because of their interesting biological properties such as anti-bacterial (Guarda *et al.*, 2003; Sabatini *et al.*, 2008), anti-fungal (Schiaffella *et al.*, 2006; Gupta & Wagh, 2006), anti-hypertensive (Cecchetti *et al.*, 2000) and anti-inflammatory (Kaneko *et al.*, 2002) activities. As a continuation of our research devoted to the development of substituted 1,4-benzothiazine derivatives (Ellouz *et al.*, 2015; Sebbar *et al.*, 2015), we report here the synthesis of the title compound by reaction of benzyl chloride with 2-(4-chlorobenzylidene)-3,4-dihydro-2*H*-1,4-benzothiazin-3-one and potassium carbonate in the presence of tetra-*n*-butylammonium bromide (as catalyst).

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C16—H16$B$···O1$^{i}$ | 0.99 | 2.43 | 3.271 (2) | 142 |

Symmetry code: (i) $-x+1, -y+2, -z+1$.

In the title compound (Fig. 1), a Cremer–Pople analysis of the conformation of the heterocyclic ring gave puckering parameters $Q$ = 0.095 (15) Å, $\theta$ = 69.3 (9)° and $\varphi$ = 233.6 (9)°. In the crystal, pairwise C16—H16$B$···O1($-x+1, -y+2, -z+1$) hydrogen bonds form dimers which stack along the $b$-axis direction (Table 1 and Fig. 2).

## Synthesis and crystallization

To a solution of 2-(4-chlorobenzylidene)-3,4-dihydro-2*H*-1,4-benzothiazin-3-one (0.944 g, 3.29 mmol), benzyl chloride (0.76 ml, 6.58 mmol) and potassium carbonate (0.91 g, 6.58 mmol) in DMF (15 ml) was added a catalytic amount of tetra-*n*-butylammonium bromide (0.11 g, 0.33 mmol). The mixture was stirred for 24 h. The solid material was removed by filtration and the solvent evaporated under vacuum. The solid product was purified by recrystallization from ethanol to afford colourless crystals in 80% yield.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Owing to poor agreement, on reflection, *i.e.* (1 1 7), was omitted from the final cycles of refinement.

## Acknowledgements

The support of NSF–MRI Grant No. 1228232 for the purchase of the diffractometer and Tulane University for support of the Tulane Crystallography Laboratory are gratefully acknowledged.

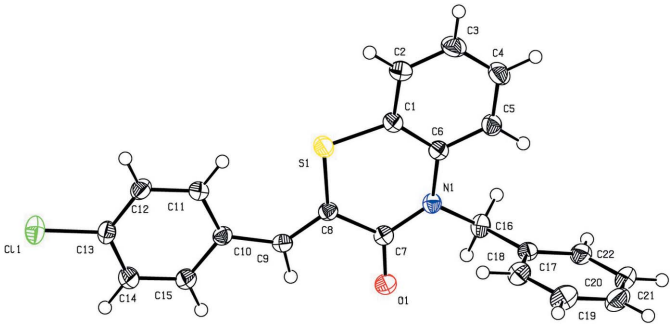



**Figure 1**
The molecular structure of the title compound, showing the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{22}H_{16}ClNOS$ |
| $M_r$ | 377.87 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 150 |
| $a, b, c$ (Å) | 11.8931 (11), 6.5358 (6), 22.817 (2) |
| $\beta$ (°) | 93.239 (1) |
| $V$ (Å$^3$) | 1770.7 (3) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.35 |
| Crystal size (mm) | 0.33 × 0.18 × 0.13 |
| | |
| Data collection | |
| Diffractometer | Bruker SMART APEX CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2016) |
| $T_{min}$, $T_{max}$ | 0.84, 0.96 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 32976, 4771, 3718 |
| $R_{int}$ | 0.047 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.686 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.044, 0.132, 1.12 |
| No. of reflections | 4771 |
| No. of parameters | 235 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 1.01, −0.47 |

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015), *SHELXL2014* (Sheldrick, 2015a), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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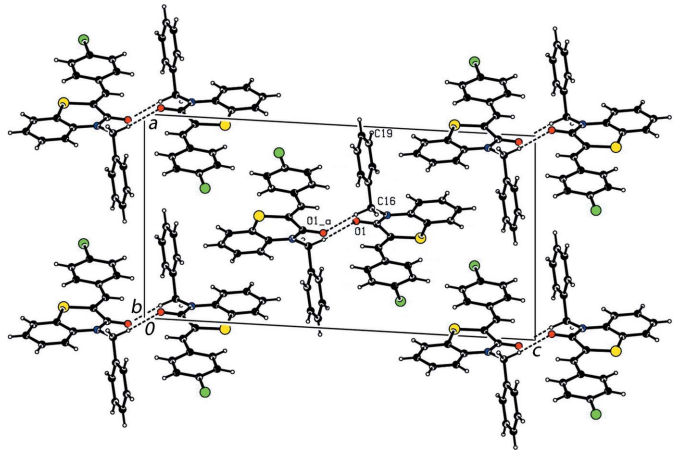


**Figure 2**
The crystal packing of the title compound, viewed along the $b$ axis. Intermolecular hydrogen bonds (see Table 2) are shown as dashed lines.

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# full crystallographic data

*IUCrData* (2016). **1**, x160764 [doi:10.1107/S2414314616007641]

## 4-Benzyl-2-(4-chlorobenzylidene)-3,4-dihydro-2*H*-1,4-benzothiazin-3(4*H*)-one

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**(2*Z*)-4-Benzyl-[(4-chlorophenyl)methylidene]-3,4-dihydro-2*H*-1,4-benzothiazin-3(4*H*)-one**

*Crystal data*

$C_{22}H_{16}ClNOS$
$M_r$ = 377.87
Monoclinic, $P2_1/n$
$a$ = 11.8931 (11) Å
$b$ = 6.5358 (6) Å
$c$ = 22.817 (2) Å
$\beta$ = 93.239 (1)°
$V$ = 1770.7 (3) Å$^3$
$Z$ = 4
$F(000)$ = 784
$D_x$ = 1.417 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9932 reflections
$\theta$ = 3.1–29.1°
$\mu$ = 0.35 mm$^{-1}$
$T$ = 150 K
Column, colourless
0.33 × 0.18 × 0.13 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
$T_{min}$ = 0.84, $T_{max}$ = 0.96
32976 measured reflections
4771 independent reflections
3718 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.047
$\theta_{max}$ = 29.2°, $\theta_{min}$ = 1.8°
$h$ = −16→16
$k$ = −8→8
$l$ = −31→31

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.132
$S$ = 1.12
4771 reflections
235 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0782P)^2 + 0.0974P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.01 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.47 e Å$^{-3}$

*Special details*

**Experimental**. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in $\omega$, collected at $\varphi$ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in $\varphi$, collected at $\omega$ = –30.00 and 210.00°. The scan time was 10 sec/frame.

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.99 Å). All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.15276 (4) | −0.28012 (7) | 0.65534 (2) | 0.03513 (14) |
| S1 | 0.46828 (4) | 0.63594 (7) | 0.70652 (2) | 0.02992 (13) |
| O1 | 0.53363 (10) | 0.75024 (19) | 0.54228 (5) | 0.0313 (3) |
| N1 | 0.57084 (10) | 0.9526 (2) | 0.62091 (5) | 0.0209 (3) |
| C1 | 0.54418 (13) | 0.8579 (2) | 0.72363 (7) | 0.0224 (3) |
| C2 | 0.56174 (14) | 0.8979 (3) | 0.78364 (7) | 0.0283 (4) |
| H2 | 0.5347 | 0.8045 | 0.8115 | 0.034* |
| C3 | 0.61815 (15) | 1.0723 (3) | 0.80268 (8) | 0.0327 (4) |
| H3 | 0.6295 | 1.0995 | 0.8435 | 0.039* |
| C4 | 0.65809 (14) | 1.2075 (3) | 0.76201 (8) | 0.0321 (4) |
| H4 | 0.6965 | 1.3282 | 0.7749 | 0.039* |
| C5 | 0.64220 (13) | 1.1672 (3) | 0.70240 (8) | 0.0264 (3) |
| H5 | 0.6708 | 1.2603 | 0.6749 | 0.032* |
| C6 | 0.58483 (12) | 0.9922 (2) | 0.68203 (7) | 0.0211 (3) |
| C7 | 0.52600 (13) | 0.7785 (2) | 0.59501 (7) | 0.0218 (3) |
| C8 | 0.46567 (12) | 0.6241 (2) | 0.63034 (7) | 0.0207 (3) |
| C9 | 0.40940 (13) | 0.4769 (2) | 0.59899 (7) | 0.0221 (3) |
| H9 | 0.4121 | 0.4924 | 0.5577 | 0.026* |
| C10 | 0.34533 (12) | 0.2989 (2) | 0.61653 (7) | 0.0218 (3) |
| C11 | 0.33017 (14) | 0.2371 (3) | 0.67448 (7) | 0.0265 (3) |
| H11 | 0.3612 | 0.3173 | 0.7061 | 0.032* |
| C12 | 0.27024 (14) | 0.0599 (3) | 0.68625 (7) | 0.0275 (4) |
| H12 | 0.2598 | 0.0205 | 0.7256 | 0.033* |
| C13 | 0.22615 (13) | −0.0581 (3) | 0.64020 (8) | 0.0255 (3) |
| C14 | 0.24071 (14) | −0.0036 (3) | 0.58230 (7) | 0.0281 (4) |
| H14 | 0.2109 | −0.0866 | 0.5510 | 0.034* |
| C15 | 0.29934 (14) | 0.1733 (3) | 0.57106 (7) | 0.0265 (3) |
| H15 | 0.3089 | 0.2115 | 0.5315 | 0.032* |
| C16 | 0.60272 (13) | 1.1156 (2) | 0.58024 (7) | 0.0246 (3) |
| H16A | 0.5719 | 1.2466 | 0.5940 | 0.029* |
| H16B | 0.5658 | 1.0866 | 0.5411 | 0.029* |
| C17 | 0.72728 (13) | 1.1438 (2) | 0.57301 (7) | 0.0222 (3) |
| C18 | 0.80536 (14) | 0.9877 (3) | 0.58319 (7) | 0.0292 (4) |
| H18 | 0.7813 | 0.8574 | 0.5960 | 0.035* |
| C19 | 0.91849 (15) | 1.0220 (3) | 0.57456 (8) | 0.0366 (4) |

| | | | | |
|---|---|---|---|---|
| H19 | 0.9716 | 0.9148 | 0.5815 | 0.044* |
| C20 | 0.95450 (16) | 1.2124 (3) | 0.55586 (9) | 0.0393 (5) |
| H20 | 1.0321 | 1.2363 | 0.5505 | 0.047* |
| C21 | 0.87698 (16) | 1.3658 (3) | 0.54511 (8) | 0.0363 (4) |
| H21 | 0.9011 | 1.4954 | 0.5317 | 0.044* |
| C22 | 0.76351 (15) | 1.3329 (3) | 0.55370 (7) | 0.0289 (4) |
| H22 | 0.7106 | 1.4401 | 0.5463 | 0.035* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0349 (2) | 0.0300 (2) | 0.0403 (3) | −0.00950 (18) | 0.00055 (18) | 0.00775 (18) |
| S1 | 0.0453 (3) | 0.0251 (2) | 0.0193 (2) | −0.01003 (18) | 0.00228 (17) | 0.00034 (15) |
| O1 | 0.0420 (7) | 0.0318 (7) | 0.0207 (6) | −0.0086 (5) | 0.0057 (5) | −0.0001 (5) |
| N1 | 0.0222 (6) | 0.0198 (7) | 0.0206 (6) | −0.0004 (5) | 0.0003 (5) | 0.0027 (5) |
| C1 | 0.0217 (7) | 0.0219 (8) | 0.0236 (7) | 0.0015 (6) | −0.0001 (6) | −0.0010 (6) |
| C2 | 0.0317 (8) | 0.0307 (9) | 0.0226 (8) | 0.0000 (7) | 0.0014 (6) | −0.0031 (7) |
| C3 | 0.0338 (9) | 0.0389 (10) | 0.0250 (8) | −0.0011 (8) | −0.0015 (7) | −0.0083 (7) |
| C4 | 0.0283 (9) | 0.0328 (9) | 0.0350 (9) | −0.0052 (7) | −0.0004 (7) | −0.0106 (8) |
| C5 | 0.0232 (8) | 0.0251 (8) | 0.0311 (8) | −0.0013 (6) | 0.0031 (6) | −0.0029 (7) |
| C6 | 0.0171 (7) | 0.0223 (8) | 0.0237 (7) | 0.0027 (6) | 0.0000 (5) | −0.0017 (6) |
| C7 | 0.0217 (7) | 0.0215 (8) | 0.0222 (7) | 0.0017 (6) | 0.0011 (6) | 0.0012 (6) |
| C8 | 0.0213 (7) | 0.0198 (7) | 0.0211 (7) | 0.0023 (6) | 0.0030 (5) | 0.0006 (6) |
| C9 | 0.0239 (7) | 0.0231 (8) | 0.0194 (7) | 0.0015 (6) | 0.0028 (6) | −0.0007 (6) |
| C10 | 0.0201 (7) | 0.0221 (8) | 0.0235 (7) | 0.0011 (6) | 0.0044 (6) | −0.0003 (6) |
| C11 | 0.0317 (8) | 0.0248 (8) | 0.0234 (8) | −0.0040 (7) | 0.0061 (6) | −0.0035 (6) |
| C12 | 0.0297 (8) | 0.0274 (9) | 0.0260 (8) | −0.0014 (7) | 0.0076 (6) | 0.0032 (6) |
| C13 | 0.0207 (7) | 0.0219 (8) | 0.0342 (9) | −0.0015 (6) | 0.0042 (6) | 0.0020 (6) |
| C14 | 0.0280 (8) | 0.0295 (9) | 0.0267 (8) | −0.0041 (7) | 0.0000 (6) | −0.0023 (7) |
| C15 | 0.0285 (8) | 0.0279 (9) | 0.0233 (8) | −0.0026 (7) | 0.0031 (6) | 0.0009 (6) |
| C16 | 0.0233 (8) | 0.0222 (8) | 0.0279 (8) | 0.0005 (6) | −0.0013 (6) | 0.0065 (6) |
| C17 | 0.0244 (7) | 0.0235 (8) | 0.0186 (7) | −0.0005 (6) | 0.0015 (5) | −0.0001 (6) |
| C18 | 0.0299 (8) | 0.0289 (9) | 0.0289 (8) | 0.0026 (7) | 0.0020 (7) | 0.0057 (7) |
| C19 | 0.0284 (9) | 0.0448 (11) | 0.0367 (10) | 0.0081 (8) | 0.0032 (7) | 0.0048 (8) |
| C20 | 0.0296 (9) | 0.0526 (12) | 0.0367 (10) | −0.0057 (9) | 0.0114 (8) | −0.0020 (9) |
| C21 | 0.0409 (10) | 0.0342 (10) | 0.0354 (10) | −0.0091 (8) | 0.0146 (8) | 0.0004 (8) |
| C22 | 0.0354 (9) | 0.0248 (8) | 0.0272 (8) | −0.0006 (7) | 0.0071 (7) | 0.0006 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C13 | 1.7383 (17) | C11—C12 | 1.394 (2) |
| S1—C8 | 1.7384 (15) | C11—H11 | 0.9500 |
| S1—C1 | 1.7409 (16) | C12—C13 | 1.383 (2) |
| O1—C7 | 1.2256 (19) | C12—H12 | 0.9500 |
| N1—C7 | 1.375 (2) | C13—C14 | 1.388 (2) |
| N1—C6 | 1.4189 (19) | C14—C15 | 1.382 (2) |
| N1—C16 | 1.4765 (19) | C14—H14 | 0.9500 |
| C1—C2 | 1.398 (2) | C15—H15 | 0.9500 |

| | | | |
|---|---|---|---|
| C1—C6 | 1.399 (2) | C16—C17 | 1.511 (2) |
| C2—C3 | 1.381 (3) | C16—H16A | 0.9900 |
| C2—H2 | 0.9500 | C16—H16B | 0.9900 |
| C3—C4 | 1.385 (3) | C17—C22 | 1.389 (2) |
| C3—H3 | 0.9500 | C17—C18 | 1.390 (2) |
| C4—C5 | 1.388 (3) | C18—C19 | 1.389 (2) |
| C4—H4 | 0.9500 | C18—H18 | 0.9500 |
| C5—C6 | 1.398 (2) | C19—C20 | 1.391 (3) |
| C5—H5 | 0.9500 | C19—H19 | 0.9500 |
| C7—C8 | 1.500 (2) | C20—C21 | 1.375 (3) |
| C8—C9 | 1.353 (2) | C20—H20 | 0.9500 |
| C9—C10 | 1.459 (2) | C21—C22 | 1.391 (2) |
| C9—H9 | 0.9500 | C21—H21 | 0.9500 |
| C10—C11 | 1.404 (2) | C22—H22 | 0.9500 |
| C10—C15 | 1.409 (2) | | |

| | | | |
|---|---|---|---|
| C8—S1—C1 | 103.94 (7) | C13—C12—C11 | 119.55 (15) |
| C7—N1—C6 | 126.48 (13) | C13—C12—H12 | 120.2 |
| C7—N1—C16 | 115.70 (13) | C11—C12—H12 | 120.2 |
| C6—N1—C16 | 117.77 (13) | C12—C13—C14 | 121.19 (15) |
| C2—C1—C6 | 120.57 (15) | C12—C13—Cl1 | 119.19 (13) |
| C2—C1—S1 | 114.98 (13) | C14—C13—Cl1 | 119.61 (13) |
| C6—C1—S1 | 124.44 (12) | C15—C14—C13 | 118.84 (16) |
| C3—C2—C1 | 120.39 (16) | C15—C14—H14 | 120.6 |
| C3—C2—H2 | 119.8 | C13—C14—H14 | 120.6 |
| C1—C2—H2 | 119.8 | C14—C15—C10 | 121.99 (15) |
| C2—C3—C4 | 119.67 (16) | C14—C15—H15 | 119.0 |
| C2—C3—H3 | 120.2 | C10—C15—H15 | 119.0 |
| C4—C3—H3 | 120.2 | N1—C16—C17 | 116.41 (13) |
| C3—C4—C5 | 120.20 (17) | N1—C16—H16A | 108.2 |
| C3—C4—H4 | 119.9 | C17—C16—H16A | 108.2 |
| C5—C4—H4 | 119.9 | N1—C16—H16B | 108.2 |
| C4—C5—C6 | 121.19 (16) | C17—C16—H16B | 108.2 |
| C4—C5—H5 | 119.4 | H16A—C16—H16B | 107.3 |
| C6—C5—H5 | 119.4 | C22—C17—C18 | 119.32 (15) |
| C5—C6—C1 | 117.97 (15) | C22—C17—C16 | 117.84 (14) |
| C5—C6—N1 | 120.27 (14) | C18—C17—C16 | 122.81 (15) |
| C1—C6—N1 | 121.75 (14) | C19—C18—C17 | 120.08 (17) |
| O1—C7—N1 | 119.88 (14) | C19—C18—H18 | 120.0 |
| O1—C7—C8 | 119.37 (14) | C17—C18—H18 | 120.0 |
| N1—C7—C8 | 120.74 (13) | C18—C19—C20 | 120.35 (17) |
| C9—C8—C7 | 115.58 (14) | C18—C19—H19 | 119.8 |
| C9—C8—S1 | 122.72 (12) | C20—C19—H19 | 119.8 |
| C7—C8—S1 | 121.71 (11) | C21—C20—C19 | 119.49 (17) |
| C8—C9—C10 | 132.25 (15) | C21—C20—H20 | 120.3 |
| C8—C9—H9 | 113.9 | C19—C20—H20 | 120.3 |
| C10—C9—H9 | 113.9 | C20—C21—C22 | 120.53 (17) |
| C11—C10—C15 | 117.47 (15) | C20—C21—H21 | 119.7 |

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| C11—C10—C9 | 125.75 (15) | C22—C21—H21 | 119.7 |
| C15—C10—C9 | 116.71 (14) | C17—C22—C21 | 120.22 (17) |
| C12—C11—C10 | 120.96 (16) | C17—C22—H22 | 119.9 |
| C12—C11—H11 | 119.5 | C21—C22—H22 | 119.9 |
| C10—C11—H11 | 119.5 | | |

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| C8—S1—C1—C2 | −177.74 (12) | C7—C8—C9—C10 | 177.40 (15) |
| C8—S1—C1—C6 | 3.15 (15) | S1—C8—C9—C10 | −2.8 (2) |
| C6—C1—C2—C3 | 0.9 (3) | C8—C9—C10—C11 | −1.7 (3) |
| S1—C1—C2—C3 | −178.23 (13) | C8—C9—C10—C15 | −178.50 (16) |
| C1—C2—C3—C4 | −0.4 (3) | C15—C10—C11—C12 | −1.0 (2) |
| C2—C3—C4—C5 | −0.4 (3) | C9—C10—C11—C12 | −177.82 (15) |
| C3—C4—C5—C6 | 0.8 (3) | C10—C11—C12—C13 | 0.7 (3) |
| C4—C5—C6—C1 | −0.3 (2) | C11—C12—C13—C14 | 0.2 (3) |
| C4—C5—C6—N1 | −179.15 (15) | C11—C12—C13—Cl1 | 179.37 (13) |
| C2—C1—C6—C5 | −0.6 (2) | C12—C13—C14—C15 | −0.8 (3) |
| S1—C1—C6—C5 | 178.50 (12) | Cl1—C13—C14—C15 | −179.96 (13) |
| C2—C1—C6—N1 | 178.28 (14) | C13—C14—C15—C10 | 0.5 (3) |
| S1—C1—C6—N1 | −2.7 (2) | C11—C10—C15—C14 | 0.4 (2) |
| C7—N1—C6—C5 | 173.47 (15) | C9—C10—C15—C14 | 177.50 (15) |
| C16—N1—C6—C5 | −9.2 (2) | C7—N1—C16—C17 | −105.82 (16) |
| C7—N1—C6—C1 | −5.4 (2) | C6—N1—C16—C17 | 76.60 (17) |
| C16—N1—C6—C1 | 171.94 (14) | N1—C16—C17—C22 | −157.04 (15) |
| C6—N1—C7—O1 | −169.28 (14) | N1—C16—C17—C18 | 24.9 (2) |
| C16—N1—C7—O1 | 13.4 (2) | C22—C17—C18—C19 | 0.6 (2) |
| C6—N1—C7—C8 | 11.9 (2) | C16—C17—C18—C19 | 178.62 (16) |
| C16—N1—C7—C8 | −165.44 (13) | C17—C18—C19—C20 | 0.1 (3) |
| O1—C7—C8—C9 | −9.2 (2) | C18—C19—C20—C21 | −1.0 (3) |
| N1—C7—C8—C9 | 169.63 (14) | C19—C20—C21—C22 | 1.0 (3) |
| O1—C7—C8—S1 | 171.00 (12) | C18—C17—C22—C21 | −0.5 (2) |
| N1—C7—C8—S1 | −10.2 (2) | C16—C17—C22—C21 | −178.64 (15) |
| C1—S1—C8—C9 | −176.80 (13) | C20—C21—C22—C17 | −0.3 (3) |
| C1—S1—C8—C7 | 2.99 (14) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C16—H16*B*···O1$^{i}$ | 0.99 | 2.43 | 3.271 (2) | 142 |

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+1.