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# (*Z*)-3-(4-Chlorophenyl)-2-(2-phenylcyclohex-2-en-1-ylimino)thiazolidin-4-one

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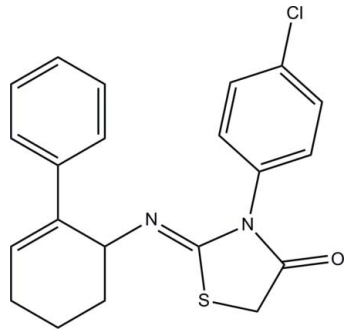
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.030; $wR$ factor = 0.083; data-to-parameter ratio = 22.3.

The title compound, $C_{21}H_{19}ClN_2OS$, exists in a *cis* conformation with respect to the N=C bond [1.2608 (13) Å]. The cyclohexene ring adopts a distorted half-chair conformation. The thiazolidine ring is close to being planar (r.m.s. deviation = 0.057 Å) and makes dihedral angles of 62.92 (6) and 56.32 (6)°, respectively, with the benzene ring and the chloro-substituted benzene ring. The dihedral angle between the benzene ring and the chloro-substituted benzene ring is 72.91 (6)°. In the crystal, molecules are linked by C—H···O and C—H···N hydrogen bonds into undulating sheets lying parallel to the *bc* plane. The crystal is further consolidated by C—H···$\pi$ interactions.

## Related literature

For details of thiazolidin-4-one derivatives, see: Previtera *et al.* (1994); Sharma *et al.* (2000); Kato *et al.* (1999*a*,*b*); Tanabe *et al.* (1991); Rawal *et al.* (2005); Voss *et al.* (2003). For related structures, see: Fun *et al.* (2011); Ooi *et al.* (2012). For ring conformations, see: Cremer & Pople (1975). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).




## Experimental

### Crystal data

$C_{21}H_{19}ClN_2OS$
$M_r$ = 382.89
Monoclinic, $P2_1/c$
$a$ = 9.1139 (3) Å
$b$ = 17.4562 (6) Å
$c$ = 12.9246 (4) Å
$\beta$ = 118.640 (2)°
$V$ = 1804.64 (10) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.34 mm$^{-1}$
$T$ = 100 K
0.37 × 0.25 × 0.18 mm

### Data collection

Bruker APEX DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.886, $T_{max}$ = 0.942
23788 measured reflections
5231 independent reflections
4605 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.083
$S$ = 1.05
5231 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

*Cg*1 is the centroid of the C1–C6 benzene ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C10—H10*A*···O1$^{i}$ | 0.99 | 2.53 | 3.4814 (17) | 161 |
| C11—H11*B*···O1$^{ii}$ | 0.99 | 2.33 | 3.2411 (14) | 152 |
| C14—H14*B*···N1$^{iii}$ | 0.99 | 2.62 | 3.4496 (14) | 141 |
| C17—H17*A*···*Cg*1$^{iv}$ | 0.95 | 2.81 | 3.5913 (13) | 140 |

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $x-1, -y-\frac{1}{2}, z-\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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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‡ Thomson Reuters ResearcherID: A-3561-2009.
§ Thomson Reuters ResearcherID: A-5525-2009.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6814).

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# supporting information

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## (*Z*)-3-(4-Chlorophenyl)-2-(2-phenylcyclohex-2-en-1-ylimino)thiazolidin-4-one

**Chin Wei Ooi, Hoong-Kun Fun, Ching Kheng Quah, Murugan Sathishkumar and Alagusundaram Ponnuswamy**

### S1. Comment

Thiazolidin-4-one derivatives are known to exhibit diverse bioactivities such as anti-histaminic (Previtera *et al.*, 1994), anti-microbial (Sharma *et al.*, 2000), (Kato *et al.*, 1999*a*), PAF antagonist (Tanabe *et al.*, 1991), cardioprotective (Kato *et al.*, 1999*b*), anti HIV (Rawal *et al.*, 2005), and tumor necrosis factor-$\alpha$ antagonist activities (Voss *et al.*, 2003).

The title compound (Fig. 1) exists in *cis* configuration with respect to the N1 ═C13 bond [N1 ═C13 = 1.2608 (13) Å]. The cyclohexene (C7–C12) ring adopts a distorted sofa conformation and the puckering parameters are Q = 0.5004 (13) Å, $\theta$ = 130.94 (15)° and $\varphi$ = 34.4 (2)° (Cremer & Pople, 1975). The thiazolidine (S1/N2/C13–C15) ring is essentially planar with a maximum deviation of 0.054 (1) Å at atom N2 and makes dihedral angles of 62.92 (6) and 56.32 (6)° respectively with the benzene ring (C1–C6) and chloro-substituted benzene ring (C16–C21). The dihedral angle between the benzene ring and chloro-substituted benzene ring is 72.91 (6)°. The bond lengths and angles are comparable to the related structures (Fun *et al.*, 2011 & Ooi *et al.*, 2012).

In the crystal structure (Fig. 2), molecules are linked *via* C10—H10A···O1, C11—H11B···O1 and C14—H14B···N1 hydrogen bonds (Table 1) into undulating sheets lying parallel to the *bc* plane. The crystal is further consolidated by C17—H17A···*Cg*1 interactions (Table 1), involving the centroid of the benzene ring (C1–C6; *Cg*1).

### S2. Experimental

A mixture of 1-(4-chlorophenyl)-3-(2-phenylcyclohex-2-enyl)thiourea (0.5 g, 2.3 mmol) and chloroacetyl chloride (0.33 g, 4.6 mmol) was heated to reflux in 1,4-dioxane (10 ml) at 100 °C for 5 h. The reaction mixture was washed with diluted sodium bicarbonate solution (25 ml) and dried over anhydrous sodium sulfate. The solvent was then evaporated under reduced pressure and the resulting residue was subjected to column chromatography using silica gel (60–120 mesh) as the stationary phase and petroleum ether-ethyl acetate (90:10) as the mobile phase to give the pure product. Yield: 0.71 g (80%); *M.p.*: 156–157 °C. Colourless blocks were obtained by recrystallization from dichloromethane solution.

### S3. Refinement

All the H atoms were positioned geometrically and refined using a riding model with $U_{iso}$(H) = 1.2 $U_{eq}$(C) (C—H = 0.95, 0.99 and 1.00 Å). In the final refinement, two outliers (1 1 7) and (-2 1 2) were omitted.

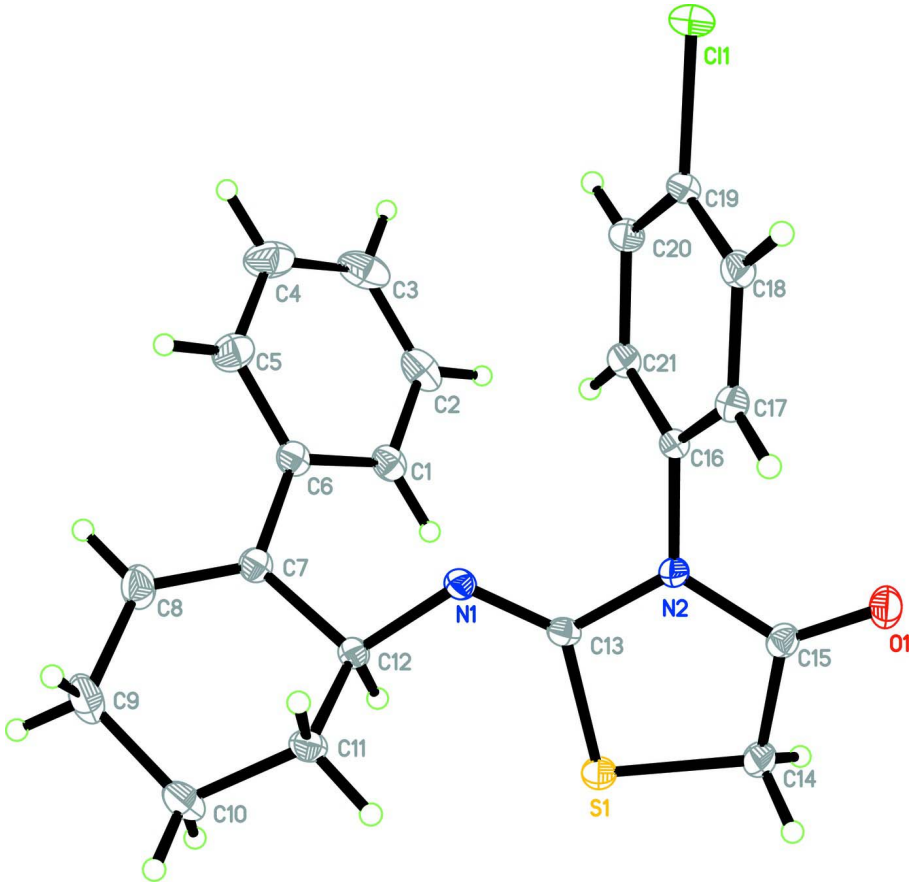


**Figure 1**

The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

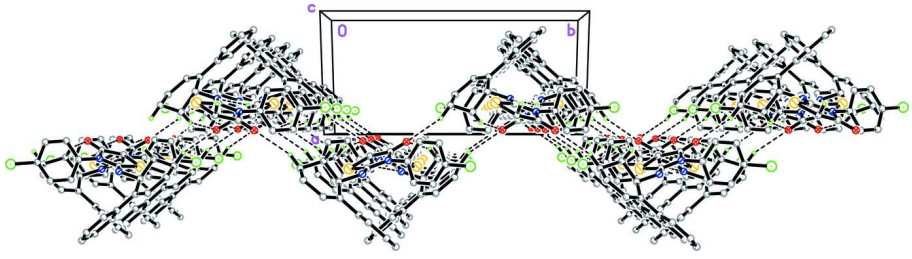


**Figure 2**

The crystal packing of the title compound, viewed along the *c* axis. H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

**(*Z*)-3-(4-Chlorophenyl)-2-(2-phenylcyclohex-2-en-1- ylimino)thiazolidin-4-one**

*Crystal data*

$C_{21}H_{19}ClN_2OS$
$M_r = 382.89$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.1139\ (3)$ Å
$b = 17.4562\ (6)$ Å
$c = 12.9246\ (4)$ Å
$\beta = 118.640\ (2)°$
$V = 1804.64\ (10)$ Å$^3$
$Z = 4$
$F(000) = 800$
$D_x = 1.409$ Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9952 reflections
$\theta$ = 2.6–34.3°
$\mu$ = 0.34 mm$^{-1}$
$T$ = 100 K
Block, colourless
0.37 × 0.25 × 0.18 mm

*Data collection*

Bruker APEX DUO CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.886, $T_{max}$ = 0.942
23788 measured reflections
5231 independent reflections
4605 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 30.0°, $\theta_{min}$ = 2.1°
$h$ = −12→12
$k$ = −24→24
$l$ = −18→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.083
$S$ = 1.05
5231 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
$w = 1/[\sigma^2(F_o^2) + (0.0385P)^2 + 0.767P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100 (1) K.

**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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.21570 (4) | −0.051642 (15) | 1.02340 (2) | 0.02160 (7) |
| S1 | 0.24459 (4) | 0.363135 (15) | 0.69867 (2) | 0.01731 (7) |
| O1 | 0.04486 (10) | 0.16687 (5) | 0.56961 (7) | 0.01895 (16) |
| N1 | 0.27625 (11) | 0.31077 (5) | 0.90882 (7) | 0.01307 (16) |
| N2 | 0.18040 (11) | 0.22633 (5) | 0.74984 (7) | 0.01253 (16) |
| C1 | 0.63915 (13) | 0.29044 (6) | 1.06753 (10) | 0.0170 (2) |
| H1A | 0.6105 | 0.3130 | 0.9933 | 0.020* |
| C2 | 0.75211 (14) | 0.22981 (7) | 1.10844 (11) | 0.0220 (2) |
| H2A | 0.7990 | 0.2111 | 1.0617 | 0.026* |
| C3 | 0.79679 (15) | 0.19637 (7) | 1.21700 (12) | 0.0277 (3) |
| H3A | 0.8734 | 0.1548 | 1.2444 | 0.033* |

| | | | | |
|---|---|---|---|---|
| C4 | 0.72833 (16) | 0.22428 (8) | 1.28510 (12) | 0.0282 (3) |
| H4A | 0.7600 | 0.2024 | 1.3602 | 0.034* |
| C5 | 0.61355 (15) | 0.28412 (7) | 1.24385 (10) | 0.0219 (2) |
| H5A | 0.5658 | 0.3019 | 1.2906 | 0.026* |
| C6 | 0.56708 (13) | 0.31871 (6) | 1.13445 (9) | 0.01562 (19) |
| C7 | 0.44377 (13) | 0.38247 (6) | 1.08949 (9) | 0.01487 (19) |
| C8 | 0.43293 (14) | 0.43351 (7) | 1.16306 (10) | 0.0214 (2) |
| H8A | 0.5073 | 0.4276 | 1.2450 | 0.026* |
| C9 | 0.31193 (16) | 0.49927 (7) | 1.12570 (11) | 0.0255 (2) |
| H9A | 0.3714 | 0.5460 | 1.1689 | 0.031* |
| H9B | 0.2233 | 0.4879 | 1.1470 | 0.031* |
| C10 | 0.23143 (15) | 0.51445 (6) | 0.99322 (11) | 0.0214 (2) |
| H10A | 0.1324 | 0.5478 | 0.9685 | 0.026* |
| H10B | 0.3120 | 0.5411 | 0.9748 | 0.026* |
| C11 | 0.17912 (13) | 0.43895 (6) | 0.92644 (9) | 0.01592 (19) |
| H11A | 0.1197 | 0.4492 | 0.8406 | 0.019* |
| H11B | 0.1013 | 0.4118 | 0.9470 | 0.019* |
| C12 | 0.33162 (13) | 0.38816 (6) | 0.95671 (9) | 0.01352 (18) |
| H12A | 0.3971 | 0.4107 | 0.9204 | 0.016* |
| C13 | 0.23863 (12) | 0.29844 (6) | 0.80285 (9) | 0.01265 (18) |
| C14 | 0.15339 (14) | 0.29402 (6) | 0.58042 (9) | 0.0176 (2) |
| H14A | 0.0486 | 0.3146 | 0.5151 | 0.021* |
| H14B | 0.2318 | 0.2828 | 0.5496 | 0.021* |
| C15 | 0.11748 (13) | 0.22186 (6) | 0.62889 (9) | 0.01409 (18) |
| C16 | 0.18581 (12) | 0.16066 (6) | 0.81802 (8) | 0.01233 (18) |
| C17 | 0.04100 (13) | 0.11881 (6) | 0.78834 (9) | 0.01434 (18) |
| H17A | −0.0632 | 0.1350 | 0.7254 | 0.017* |
| C18 | 0.05075 (14) | 0.05291 (6) | 0.85211 (9) | 0.01572 (19) |
| H18A | −0.0464 | 0.0232 | 0.8324 | 0.019* |
| C19 | 0.20399 (14) | 0.03118 (6) | 0.94472 (9) | 0.01523 (19) |
| C20 | 0.34831 (13) | 0.07366 (6) | 0.97650 (9) | 0.01584 (19) |
| H20A | 0.4516 | 0.0586 | 1.0415 | 0.019* |
| C21 | 0.33872 (13) | 0.13850 (6) | 0.91151 (9) | 0.01426 (18) |
| H21A | 0.4364 | 0.1678 | 0.9308 | 0.017* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.02893 (14) | 0.01406 (12) | 0.02091 (13) | 0.00025 (10) | 0.01122 (11) | 0.00494 (9) |
| S1 | 0.02495 (14) | 0.01306 (12) | 0.01514 (12) | −0.00279 (9) | 0.01059 (10) | 0.00118 (9) |
| O1 | 0.0237 (4) | 0.0184 (4) | 0.0148 (3) | −0.0037 (3) | 0.0093 (3) | −0.0040 (3) |
| N1 | 0.0136 (4) | 0.0108 (4) | 0.0129 (4) | −0.0009 (3) | 0.0049 (3) | −0.0001 (3) |
| N2 | 0.0156 (4) | 0.0107 (4) | 0.0104 (4) | −0.0015 (3) | 0.0054 (3) | 0.0001 (3) |
| C1 | 0.0138 (4) | 0.0152 (5) | 0.0193 (5) | −0.0023 (4) | 0.0058 (4) | −0.0026 (4) |
| C2 | 0.0135 (5) | 0.0173 (5) | 0.0327 (6) | −0.0014 (4) | 0.0090 (4) | −0.0048 (4) |
| C3 | 0.0154 (5) | 0.0196 (6) | 0.0383 (7) | 0.0030 (4) | 0.0051 (5) | 0.0053 (5) |
| C4 | 0.0227 (6) | 0.0273 (6) | 0.0253 (6) | 0.0023 (5) | 0.0041 (5) | 0.0089 (5) |
| C5 | 0.0188 (5) | 0.0248 (6) | 0.0184 (5) | 0.0007 (4) | 0.0059 (4) | 0.0025 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.0122 (4) | 0.0149 (5) | 0.0157 (4) | −0.0018 (4) | 0.0034 (4) | −0.0015 (4) |
| C7 | 0.0127 (4) | 0.0149 (5) | 0.0143 (4) | −0.0010 (4) | 0.0043 (4) | −0.0012 (4) |
| C8 | 0.0194 (5) | 0.0224 (5) | 0.0171 (5) | 0.0011 (4) | 0.0045 (4) | −0.0055 (4) |
| C9 | 0.0251 (6) | 0.0211 (6) | 0.0260 (6) | 0.0029 (5) | 0.0088 (5) | −0.0091 (4) |
| C10 | 0.0212 (5) | 0.0129 (5) | 0.0277 (6) | 0.0013 (4) | 0.0096 (4) | −0.0018 (4) |
| C11 | 0.0156 (4) | 0.0126 (4) | 0.0164 (4) | 0.0015 (4) | 0.0050 (4) | 0.0015 (4) |
| C12 | 0.0148 (4) | 0.0107 (4) | 0.0133 (4) | −0.0016 (3) | 0.0053 (4) | −0.0008 (3) |
| C13 | 0.0126 (4) | 0.0107 (4) | 0.0139 (4) | −0.0001 (3) | 0.0057 (3) | 0.0013 (3) |
| C14 | 0.0244 (5) | 0.0163 (5) | 0.0137 (4) | −0.0018 (4) | 0.0103 (4) | 0.0002 (4) |
| C15 | 0.0150 (4) | 0.0160 (5) | 0.0124 (4) | 0.0007 (4) | 0.0075 (4) | −0.0002 (3) |
| C16 | 0.0154 (4) | 0.0103 (4) | 0.0113 (4) | 0.0003 (3) | 0.0064 (3) | −0.0002 (3) |
| C17 | 0.0145 (4) | 0.0146 (4) | 0.0122 (4) | −0.0008 (4) | 0.0050 (3) | −0.0008 (3) |
| C18 | 0.0176 (5) | 0.0144 (5) | 0.0149 (4) | −0.0038 (4) | 0.0076 (4) | −0.0019 (4) |
| C19 | 0.0222 (5) | 0.0100 (4) | 0.0143 (4) | 0.0010 (4) | 0.0093 (4) | 0.0008 (3) |
| C20 | 0.0162 (4) | 0.0142 (5) | 0.0153 (4) | 0.0034 (4) | 0.0061 (4) | 0.0008 (4) |
| C21 | 0.0133 (4) | 0.0132 (4) | 0.0156 (4) | −0.0001 (3) | 0.0064 (4) | −0.0009 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C19 | 1.7411 (11) | C8—H8A | 0.9500 |
| S1—C13 | 1.7780 (10) | C9—C10 | 1.5284 (18) |
| S1—C14 | 1.8067 (11) | C9—H9A | 0.9900 |
| O1—C15 | 1.2084 (13) | C9—H9B | 0.9900 |
| N1—C13 | 1.2608 (13) | C10—C11 | 1.5215 (15) |
| N1—C12 | 1.4707 (13) | C10—H10A | 0.9900 |
| N2—C15 | 1.3854 (12) | C10—H10B | 0.9900 |
| N2—C13 | 1.4096 (13) | C11—C12 | 1.5329 (14) |
| N2—C16 | 1.4322 (13) | C11—H11A | 0.9900 |
| C1—C2 | 1.3921 (15) | C11—H11B | 0.9900 |
| C1—C6 | 1.4027 (15) | C12—H12A | 1.0000 |
| C1—H1A | 0.9500 | C14—C15 | 1.5110 (15) |
| C2—C3 | 1.3883 (19) | C14—H14A | 0.9900 |
| C2—H2A | 0.9500 | C14—H14B | 0.9900 |
| C3—C4 | 1.388 (2) | C16—C17 | 1.3920 (14) |
| C3—H3A | 0.9500 | C16—C21 | 1.3920 (14) |
| C4—C5 | 1.3911 (17) | C17—C18 | 1.3929 (14) |
| C4—H4A | 0.9500 | C17—H17A | 0.9500 |
| C5—C6 | 1.4032 (15) | C18—C19 | 1.3873 (15) |
| C5—H5A | 0.9500 | C18—H18A | 0.9500 |
| C6—C7 | 1.4878 (15) | C19—C20 | 1.3895 (15) |
| C7—C8 | 1.3408 (15) | C20—C21 | 1.3871 (14) |
| C7—C12 | 1.5226 (14) | C20—H20A | 0.9500 |
| C8—C9 | 1.5021 (17) | C21—H21A | 0.9500 |
| | | | |
| C13—S1—C14 | 92.74 (5) | C10—C11—H11A | 109.5 |
| C13—N1—C12 | 118.28 (9) | C12—C11—H11A | 109.5 |
| C15—N2—C13 | 117.03 (8) | C10—C11—H11B | 109.5 |
| C15—N2—C16 | 121.51 (8) | C12—C11—H11B | 109.5 |

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| C13—N2—C16 | 121.45 (8) | H11A—C11—H11B | 108.0 |
| C2—C1—C6 | 120.85 (11) | N1—C12—C7 | 108.91 (8) |
| C2—C1—H1A | 119.6 | N1—C12—C11 | 109.73 (8) |
| C6—C1—H1A | 119.6 | C7—C12—C11 | 111.23 (8) |
| C3—C2—C1 | 120.59 (11) | N1—C12—H12A | 109.0 |
| C3—C2—H2A | 119.7 | C7—C12—H12A | 109.0 |
| C1—C2—H2A | 119.7 | C11—C12—H12A | 109.0 |
| C2—C3—C4 | 119.33 (11) | N1—C13—N2 | 121.56 (9) |
| C2—C3—H3A | 120.3 | N1—C13—S1 | 128.54 (8) |
| C4—C3—H3A | 120.3 | N2—C13—S1 | 109.89 (7) |
| C3—C4—C5 | 120.29 (12) | C15—C14—S1 | 108.01 (7) |
| C3—C4—H4A | 119.9 | C15—C14—H14A | 110.1 |
| C5—C4—H4A | 119.9 | S1—C14—H14A | 110.1 |
| C4—C5—C6 | 121.17 (12) | C15—C14—H14B | 110.1 |
| C4—C5—H5A | 119.4 | S1—C14—H14B | 110.1 |
| C6—C5—H5A | 119.4 | H14A—C14—H14B | 108.4 |
| C1—C6—C5 | 117.75 (10) | O1—C15—N2 | 124.39 (10) |
| C1—C6—C7 | 120.77 (10) | O1—C15—C14 | 124.13 (9) |
| C5—C6—C7 | 121.48 (10) | N2—C15—C14 | 111.47 (9) |
| C8—C7—C6 | 121.25 (10) | C17—C16—C21 | 121.06 (9) |
| C8—C7—C12 | 121.21 (10) | C17—C16—N2 | 120.14 (9) |
| C6—C7—C12 | 117.54 (9) | C21—C16—N2 | 118.78 (9) |
| C7—C8—C9 | 124.89 (10) | C16—C17—C18 | 119.16 (9) |
| C7—C8—H8A | 117.6 | C16—C17—H17A | 120.4 |
| C9—C8—H8A | 117.6 | C18—C17—H17A | 120.4 |
| C8—C9—C10 | 112.15 (10) | C19—C18—C17 | 119.25 (10) |
| C8—C9—H9A | 109.2 | C19—C18—H18A | 120.4 |
| C10—C9—H9A | 109.2 | C17—C18—H18A | 120.4 |
| C8—C9—H9B | 109.2 | C18—C19—C20 | 121.87 (10) |
| C10—C9—H9B | 109.2 | C18—C19—Cl1 | 119.04 (8) |
| H9A—C9—H9B | 107.9 | C20—C19—Cl1 | 119.09 (8) |
| C11—C10—C9 | 109.69 (10) | C21—C20—C19 | 118.72 (10) |
| C11—C10—H10A | 109.7 | C21—C20—H20A | 120.6 |
| C9—C10—H10A | 109.7 | C19—C20—H20A | 120.6 |
| C11—C10—H10B | 109.7 | C20—C21—C16 | 119.91 (10) |
| C9—C10—H10B | 109.7 | C20—C21—H21A | 120.0 |
| H10A—C10—H10B | 108.2 | C16—C21—H21A | 120.0 |
| C10—C11—C12 | 110.92 (9) | | |

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| C6—C1—C2—C3 | −0.49 (17) | C15—N2—C13—N1 | 170.00 (9) |
| C1—C2—C3—C4 | −0.36 (18) | C16—N2—C13—N1 | −9.89 (15) |
| C2—C3—C4—C5 | 1.30 (19) | C15—N2—C13—S1 | −9.15 (11) |
| C3—C4—C5—C6 | −1.42 (19) | C16—N2—C13—S1 | 170.96 (7) |
| C2—C1—C6—C5 | 0.38 (16) | C14—S1—C13—N1 | −175.13 (10) |
| C2—C1—C6—C7 | −178.76 (10) | C14—S1—C13—N2 | 3.95 (8) |
| C4—C5—C6—C1 | 0.56 (17) | C13—S1—C14—C15 | 1.41 (8) |
| C4—C5—C6—C7 | 179.69 (11) | C13—N2—C15—O1 | −170.49 (10) |
| C1—C6—C7—C8 | −147.73 (11) | C16—N2—C15—O1 | 9.40 (16) |

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| C5—C6—C7—C8 | 33.17 (16) | C13—N2—C15—C14 | 10.39 (13) |
| C1—C6—C7—C12 | 31.62 (14) | C16—N2—C15—C14 | −169.72 (9) |
| C5—C6—C7—C12 | −147.49 (10) | S1—C14—C15—O1 | 174.28 (9) |
| C6—C7—C8—C9 | −179.63 (11) | S1—C14—C15—N2 | −6.60 (11) |
| C12—C7—C8—C9 | 1.05 (18) | C15—N2—C16—C17 | −54.52 (13) |
| C7—C8—C9—C10 | −14.39 (18) | C13—N2—C16—C17 | 125.37 (10) |
| C8—C9—C10—C11 | 44.28 (14) | C15—N2—C16—C21 | 123.55 (10) |
| C9—C10—C11—C12 | −63.22 (12) | C13—N2—C16—C21 | −56.56 (13) |
| C13—N1—C12—C7 | −153.55 (9) | C21—C16—C17—C18 | −1.28 (15) |
| C13—N1—C12—C11 | 84.48 (11) | N2—C16—C17—C18 | 176.74 (9) |
| C8—C7—C12—N1 | −139.34 (11) | C16—C17—C18—C19 | 0.93 (15) |
| C6—C7—C12—N1 | 41.32 (12) | C17—C18—C19—C20 | 0.53 (16) |
| C8—C7—C12—C11 | −18.28 (14) | C17—C18—C19—Cl1 | −179.52 (8) |
| C6—C7—C12—C11 | 162.38 (9) | C18—C19—C20—C21 | −1.63 (16) |
| C10—C11—C12—N1 | 169.61 (9) | Cl1—C19—C20—C21 | 178.41 (8) |
| C10—C11—C12—C7 | 49.04 (12) | C19—C20—C21—C16 | 1.27 (15) |
| C12—N1—C13—N2 | −178.32 (9) | C17—C16—C21—C20 | 0.16 (15) |
| C12—N1—C13—S1 | 0.66 (14) | N2—C16—C21—C20 | −177.89 (9) |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C1–C6 benzene ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C10—H10*A*···O1$^{i}$ | 0.99 | 2.53 | 3.4814 (17) | 161 |
| C11—H11*B*···O1$^{ii}$ | 0.99 | 2.33 | 3.2411 (14) | 152 |
| C14—H14*B*···N1$^{iii}$ | 0.99 | 2.62 | 3.4496 (14) | 141 |
| C17—H17*A*···*Cg*1$^{iv}$ | 0.95 | 2.81 | 3.5913 (13) | 140 |

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