

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

Chin Wei Ooi,^a Hoong-Kun Fun,^{a*} ‡ Ching Kheng Quah,^{a§} Murugan Sathishkumar^b and Alagusundaram Ponnuswamy^b

^aX-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and ^bDepartment of Organic Chemistry, School of Chemistry, Madurai Kamaraj University, Madurai 625 021, Tamil Nadu, India
Correspondence e-mail: hkfun@usm.my

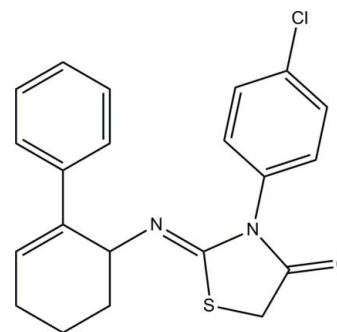
Received 22 May 2012; accepted 28 May 2012

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

The title compound, $\text{C}_{21}\text{H}_{19}\text{ClN}_2\text{OS}$, exists in a *cis* conformation with respect to the $\text{N}=\text{C}$ 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 $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds into undulating sheets lying parallel to the *bc* plane. The crystal is further consolidated by $\text{C}-\text{H}\cdots\pi$ interactions.

Related literature

For details of thiazolidin-4-one derivatives, see: Previtiera *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

$\text{C}_{21}\text{H}_{19}\text{ClN}_2\text{OS}$	$V = 1804.64 (10) \text{ \AA}^3$
$M_r = 382.89$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 9.1139 (3) \text{ \AA}$	$\mu = 0.34 \text{ mm}^{-1}$
$b = 17.4562 (6) \text{ \AA}$	$T = 100 \text{ K}$
$c = 12.9246 (4) \text{ \AA}$	$0.37 \times 0.25 \times 0.18 \text{ mm}$
$\beta = 118.640 (2)^\circ$	

Data collection

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

Refinement

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

Table 1

Hydrogen-bond geometry (Å, °).

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

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C10}-\text{H10A}\cdots\text{O1}^{\text{i}}$	0.99	2.53	3.4814 (17)	161
$\text{C11}-\text{H11B}\cdots\text{O1}^{\text{ii}}$	0.99	2.33	3.2411 (14)	152
$\text{C14}-\text{H14B}\cdots\text{N1}^{\text{iii}}$	0.99	2.62	3.4496 (14)	141
$\text{C17}-\text{H17A}\cdots\text{Cg1}^{\text{iv}}$	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).

CWO, HKF and CKQ thank Universiti Sains Malaysia (USM) for the Research University Grant (1001/PFIZIK/811160). CWO also thanks the Malaysian Government and USM for the award of the post of Research Officer under Research University Grant No. 1001/PFIZIK/811160.

‡ 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).

References

- Bruker (2009). *SADABS*, *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
- Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
- Fun, H.-K., Hemamalini, M., Shanmugavelan, P., Ponnuswamy, A. & Jagatheesan, R. (2011). *Acta Cryst.* **E67**, o2706.
- Kato, T., Ozaki, T. & Ohi, N. (1999*b*). *Tetrahedron Asymmetry*, **10**, 3963–3968.
- Kato, T., Ozaki, T. & Tamura, K. (1999*a*). *J. Med. Chem.* **42**, 3134–3146.
- Ooi, C. W., Fun, H.-K., Quah, C. K., Sathishkumar, M. & Ponnuswamy, A. (2012). *Acta Cryst.* **E68**, o1796–o1797.
- Previtera, T., Vigorita, M. G., Bisila, M., Orsini, F., Benetolla, F. & Bombieri, G. (1994). *Eur. J. Med. Chem.* **29**, 317–324.
- Rawal, R. K., Prabhakar, Y. S., Katti, S. B. & De Clercq, E. (2005). *Bioorg. Med. Chem.* **13**, 6771–6776.
- Sharma, R. C. & Kumar, D. (2000). *J. Indian Chem. Soc.* **77**, 492–493.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Tanabe, Y., Suzukamo, G., Komuro, Y., Imanishi, N., Morooka, S., Enomoto, M., Kojima, A., Sanemitsu, Y. & Mizutani, M. (1991). *Tetrahedron Lett.* **32**, 379–382.
- Voss, M. E., Carter, P. H., Tebben, A. J., Scherle, P. A., Brown, G. D. & Thompson, L. A. (2003). *Bioorg. Med. Chem. Lett.* **13**, 533–538.

supplementary materials

Acta Cryst. (2012). E68, o1999–o2000 [doi:10.1107/S1600536812024294]

(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

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.*, 1999a), PAF antagonist (Tanabe *et al.*, 1991), cardioprotective (Kato *et al.*, 1999b), anti HIV (Rawal *et al.*, 2005), and tumor necrosis factor- α 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···Cg1 interactions (Table 1), involving the centroid of the benzene ring (C1–C6; Cg1).

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.

Refinement

All the H atoms were positioned geometrically and refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ (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.

Computing details

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

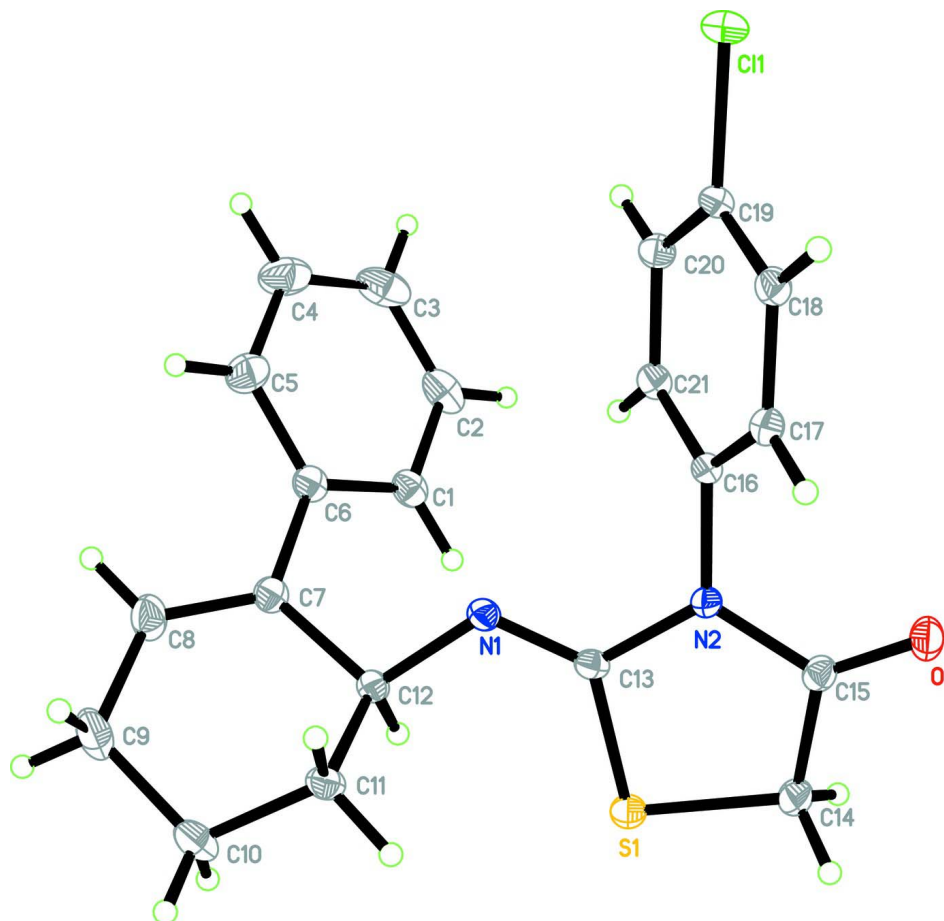


Figure 1

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

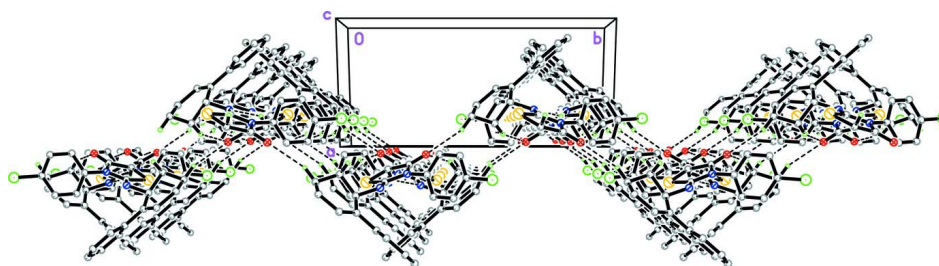


Figure 2

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: $-P\ 2_1/c$

$a = 9.1139\ (3)\ \text{\AA}$

$b = 17.4562\ (6)\ \text{\AA}$

$c = 12.9246\ (4)\ \text{\AA}$

$\beta = 118.640\ (2)^\circ$

$V = 1804.64\ (10)\ \text{\AA}^3$

$Z = 4$

$F(000) = 800$
 $D_x = 1.409 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 9952 reflections
 $\theta = 2.6\text{--}34.3^\circ$

$\mu = 0.34 \text{ mm}^{-1}$
 $T = 100 \text{ K}$
 Block, colourless
 $0.37 \times 0.25 \times 0.18 \text{ mm}$

Data collection

Bruker APEX DUO CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\text{max}} = 30.0^\circ$, $\theta_{\text{min}} = 2.1^\circ$
 $h = -12 \rightarrow 12$
 $k = -24 \rightarrow 24$
 $l = -18 \rightarrow 18$

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 $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.42 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^2)

	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, °)

C11—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
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—C11	119.04 (8)
H9A—C9—H9B	107.9	C20—C19—C11	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)		
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)
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—C11	-179.52 (8)
C6—C7—C12—C11	162.38 (9)	C18—C19—C20—C21	-1.63 (16)
C10—C11—C12—N1	169.61 (9)	C11—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, °)

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

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C10—H10 <i>A</i> ...O1 ⁱ	0.99	2.53	3.4814 (17)	161
C11—H11 <i>B</i> ...O1 ⁱⁱ	0.99	2.33	3.2411 (14)	152
C14—H14 <i>B</i> ...N1 ⁱⁱⁱ	0.99	2.62	3.4496 (14)	141
C17—H17 <i>A</i> ...Cg1 ^{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) $x-1, -y-1/2, z-3/2$.