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## Structure Reports

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**(Z)-3-*p*-Tolyl-2-(*p*-tolylimino)-1,3-thiazolidin-4-one**Hatem A. Abdel-Aziz,<sup>a</sup> Hazem A. Ghabbour,<sup>a</sup> Tze Shyang Chia<sup>b</sup> and Hoong-Kun Fun<sup>b\*</sup>†<sup>a</sup>Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, PO Box 2457, Riyadh 11451, Saudi Arabia, and <sup>b</sup>X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia  
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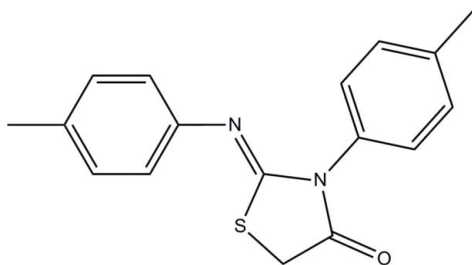
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.046;  $wR$  factor = 0.135; data-to-parameter ratio = 14.7.

In the title compound,  $\text{C}_{17}\text{H}_{16}\text{N}_2\text{OS}$ , the central thiazolidin-4-one ring forms dihedral angles of 66.49 (9) and 79.45 (6)° with the two methyl-substituted benzene rings. In the crystal, molecules are stacked in columns along the  $b$  axis through  $\text{C}-\text{H}\cdots\pi$  interactions. The H atoms of one of the methyl groups are disordered over two orientations with equal site occupancies.

## Related literature

For the chemistry of thiazolidin-4-one and its experimental preparation, see: Abdel-Aziz *et al.* (2010). For a related structure, see: Zeller *et al.* (2011). For reference bond lengths, see: Allen *et al.* (1987).



## Experimental

## Crystal data

 $\text{C}_{17}\text{H}_{16}\text{N}_2\text{OS}$   
 $M_r = 296.38$   
Monoclinic,  $P2_1/c$  $a = 14.1321$  (4) Å  
 $b = 5.8524$  (2) Å  
 $c = 19.0076$  (6) Å $\beta = 100.307$  (2)°  
 $V = 1546.69$  (8) Å<sup>3</sup>  
 $Z = 4$   
Cu  $K\alpha$  radiation $\mu = 1.85$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.98 \times 0.21 \times 0.06$  mm

## Data collection

Bruker SMART APEXII CCD  
area-detector diffractometer  
Absorption correction: multi-scan  
(SADABS; Bruker, 2009)  
 $T_{\min} = 0.264$ ,  $T_{\max} = 0.897$ 10830 measured reflections  
2849 independent reflections  
2293 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.041$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.135$   
 $S = 1.07$   
2849 reflections194 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.35$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.35$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

 $\text{Cg1}$  and  $\text{Cg2}$  are the centroids of the  $\text{S1/N2/C1}-\text{C3}$  and  $\text{C4}-\text{C9}$  rings, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C5}-\text{H5A}\cdots\text{Cg1}^i$	0.93	3.00	3.788 (2)	144
$\text{C9}-\text{H9A}\cdots\text{Cg2}^{ii}$	0.93	2.87	3.607 (2)	138

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

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5090).

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† Thomson Reuters ResearcherID: A-3561-2009.

## supplementary materials

*Acta Cryst.* (2012). E68, o1143 [doi:10.1107/S160053681201149X]

**(Z)-3-*p*-Tolyl-2-(*p*-tolylimino)-1,3-thiazolidin-4-one****Hatem A. Abdel-Aziz, Hazem A. Ghabbour, Tze Shyang Chia and Hoong-Kun Fun****Comment**

The molecular structure of the title compound is shown in Fig. 1. The mean planes of the two methyl-substituted benzene rings (C4–C9 & C10–C15) make dihedral angles of 66.49 (9) and 79.45 (6)°, respectively, with the mean plane of the central thiazolidin-4-one ring [S1/N2/C1–C3/O1; maximum deviation = 0.0075 (12) Å at atom C3]. In the molecule, the hydrogen atoms which are attached to atom C17 are disordered over two positions, with equal site-occupancies. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and are comparable to a related structure (Zeller *et al.*, 2011).

In the crystal structure, no significant intermolecular hydrogen bonds are observed. The crystal structure is stabilized by C—H... $\pi$  interactions (Table 1), involving Cg1 and Cg2 which are the centroids of S1/N2/C1–C3 and C4–C9 rings, respectively.

**Experimental**

The title compound was prepared according to the reported method by Abdel-Aziz *et al.* (2010). Crystals of the title compound were obtained by slow evaporation from an ethanol solution at room temperature.

**Refinement**

The methyl group with atom C17 was found to be disordered over two orientations and the H atoms were located in a difference Fourier map. The site-occupancy ratio was refined to 0.52 (3):0.48 (3) in the refinement using C—H bond distance restraints. In the final refinement, the occupancies were fixed at 0.5 and the H atoms were treated as riding (C—H = 0.96 Å), with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ . A rotating group model was used for each of the disordered components. All other H atoms were positioned geometrically (C—H = 0.93, 0.96 or 0.97 Å) and refined using a riding model with  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5U_{\text{eq}}(\text{C})$ . A rotating group model was also applied to the other methyl group.

**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).

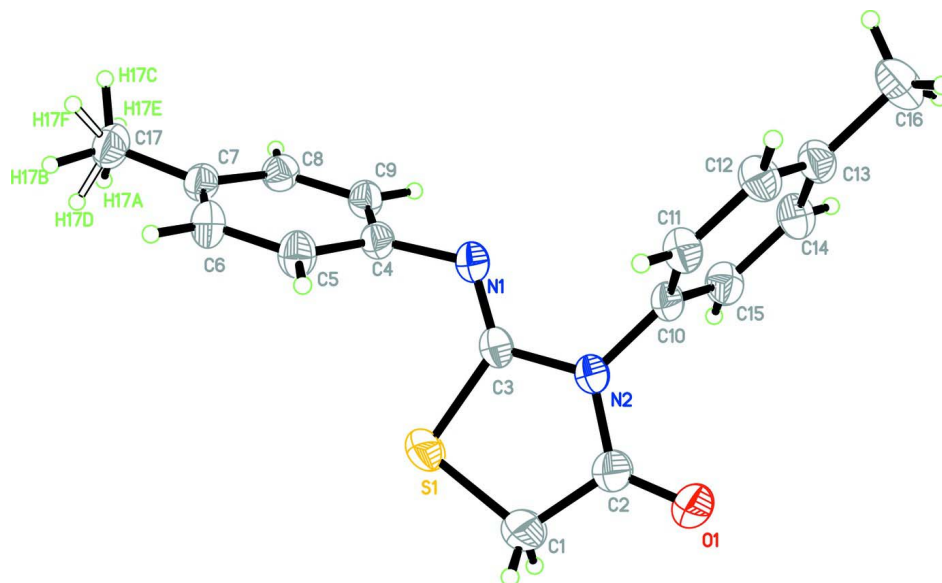


Figure 1

The molecular structure of the title compound with atom labels and 30% probability displacement ellipsoids.

**(Z)-3-*p*-Tolyl-2-(*p*-tolylimino)-1,3-thiazolidin-4-one**

*Crystal data*

$C_{17}H_{16}N_2OS$

$M_r = 296.38$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 14.1321(4) \text{ \AA}$

$b = 5.8524(2) \text{ \AA}$

$c = 19.0076(6) \text{ \AA}$

$\beta = 100.307(2)^\circ$

$V = 1546.69(8) \text{ \AA}^3$

$Z = 4$

$F(000) = 624$

$D_x = 1.273 \text{ Mg m}^{-3}$

Cu  $K\alpha$  radiation,  $\lambda = 1.54178 \text{ \AA}$

Cell parameters from 1135 reflections

$\theta = 4.7\text{--}69.2^\circ$

$\mu = 1.85 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Needle, colourless

$0.98 \times 0.21 \times 0.06 \text{ mm}$

*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, 2009)

$T_{\min} = 0.264$ ,  $T_{\max} = 0.897$

10830 measured reflections

2849 independent reflections

2293 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$

$\theta_{\max} = 69.8^\circ$ ,  $\theta_{\min} = 4.7^\circ$

$h = -16 \rightarrow 17$

$k = -5 \rightarrow 6$

$l = -23 \rightarrow 22$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.135$

$S = 1.07$

2849 reflections

194 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 0.2896P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.35 \text{ e } \text{Å}^{-3}$

$\Delta\rho_{\min} = -0.35 \text{ e } \text{Å}^{-3}$   
 Extinction correction: *SHELXTL* (Sheldrick, 2008),  $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.0124 (10)

*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 ( $\text{Å}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
S1	0.86258 (4)	−0.00010 (12)	0.47164 (3)	0.0765 (3)	
N1	0.84789 (10)	−0.0771 (3)	0.32906 (8)	0.0522 (4)	
N2	0.73053 (10)	0.1441 (3)	0.36745 (8)	0.0523 (4)	
O1	0.63384 (14)	0.3619 (4)	0.42357 (10)	0.1118 (8)	
C1	0.7698 (2)	0.1807 (7)	0.49367 (13)	0.1031 (11)	
H1A	0.7349	0.1019	0.5260	0.124*	
H1B	0.7977	0.3185	0.5171	0.124*	
C2	0.70278 (16)	0.2406 (5)	0.42561 (12)	0.0757 (7)	
C3	0.81438 (12)	0.0103 (3)	0.37930 (10)	0.0496 (4)	
C4	0.93412 (12)	−0.2091 (3)	0.34399 (9)	0.0479 (4)	
C5	0.93843 (14)	−0.4167 (3)	0.37968 (12)	0.0584 (5)	
H5A	0.8857	−0.4678	0.3983	0.070*	
C6	1.02137 (14)	−0.5478 (3)	0.38750 (12)	0.0591 (5)	
H6A	1.0236	−0.6864	0.4117	0.071*	
C7	1.10064 (13)	−0.4772 (3)	0.36010 (11)	0.0515 (5)	
C8	1.09587 (13)	−0.2684 (3)	0.32587 (10)	0.0530 (4)	
H8A	1.1492	−0.2155	0.3083	0.064*	
C9	1.01362 (13)	−0.1362 (3)	0.31707 (10)	0.0514 (4)	
H9A	1.0117	0.0025	0.2929	0.062*	
C10	0.67884 (12)	0.1860 (3)	0.29574 (10)	0.0475 (4)	
C11	0.61531 (13)	0.0238 (3)	0.26253 (11)	0.0535 (5)	
H11A	0.6064	−0.1124	0.2857	0.064*	
C12	0.56500 (14)	0.0659 (4)	0.19452 (11)	0.0584 (5)	
H12A	0.5222	−0.0434	0.1721	0.070*	
C13	0.57711 (13)	0.2673 (4)	0.15916 (10)	0.0561 (5)	
C14	0.64077 (14)	0.4275 (4)	0.19421 (11)	0.0592 (5)	
H14A	0.6495	0.5644	0.1714	0.071*	
C15	0.69157 (13)	0.3888 (3)	0.26226 (11)	0.0563 (5)	
H15A	0.7338	0.4986	0.2851	0.068*	
C16	0.52221 (18)	0.3121 (5)	0.08465 (13)	0.0838 (8)	
H16A	0.4567	0.2639	0.0816	0.126*	
H16B	0.5512	0.2284	0.0506	0.126*	

H16C	0.5239	0.4725	0.0744	0.126*	
C17	1.18878 (15)	-0.6264 (4)	0.36447 (13)	0.0688 (6)	
H17A	1.2442	-0.5449	0.3885	0.103*	0.50
H17B	1.1977	-0.6659	0.3171	0.103*	0.50
H17C	1.1804	-0.7631	0.3906	0.103*	0.50
H17D	1.2256	-0.6203	0.4120	0.103*	0.50
H17E	1.2273	-0.5724	0.3311	0.103*	0.50
H17F	1.1694	-0.7811	0.3530	0.103*	0.50

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0617 (4)	0.1143 (5)	0.0480 (4)	0.0285 (3)	-0.0047 (2)	0.0048 (3)
N1	0.0461 (8)	0.0559 (9)	0.0516 (9)	0.0101 (7)	0.0007 (6)	0.0030 (7)
N2	0.0441 (8)	0.0635 (10)	0.0461 (8)	0.0110 (7)	-0.0010 (6)	-0.0011 (7)
O1	0.0957 (13)	0.165 (2)	0.0691 (11)	0.0751 (14)	-0.0007 (9)	-0.0207 (12)
C1	0.0900 (18)	0.159 (3)	0.0529 (13)	0.0537 (19)	-0.0063 (12)	-0.0151 (16)
C2	0.0616 (12)	0.1040 (18)	0.0575 (12)	0.0279 (13)	-0.0003 (10)	-0.0105 (12)
C3	0.0412 (9)	0.0541 (10)	0.0502 (10)	0.0044 (7)	-0.0009 (8)	0.0044 (8)
C4	0.0464 (9)	0.0470 (9)	0.0472 (9)	0.0061 (7)	0.0003 (7)	-0.0010 (7)
C5	0.0487 (10)	0.0565 (11)	0.0701 (13)	0.0018 (8)	0.0110 (9)	0.0098 (9)
C6	0.0561 (11)	0.0474 (11)	0.0718 (13)	0.0066 (8)	0.0062 (9)	0.0119 (9)
C7	0.0491 (10)	0.0494 (10)	0.0530 (10)	0.0064 (7)	0.0013 (8)	-0.0053 (8)
C8	0.0492 (9)	0.0546 (11)	0.0550 (10)	0.0001 (8)	0.0092 (8)	-0.0027 (8)
C9	0.0559 (10)	0.0455 (10)	0.0516 (10)	0.0038 (8)	0.0061 (8)	0.0039 (7)
C10	0.0377 (8)	0.0539 (10)	0.0477 (9)	0.0077 (7)	-0.0010 (7)	-0.0008 (7)
C11	0.0495 (10)	0.0507 (10)	0.0573 (11)	-0.0010 (7)	0.0017 (8)	0.0047 (8)
C12	0.0487 (10)	0.0642 (12)	0.0575 (11)	-0.0066 (8)	-0.0030 (8)	-0.0023 (9)
C13	0.0456 (9)	0.0677 (12)	0.0524 (11)	0.0038 (8)	0.0017 (8)	0.0036 (9)
C14	0.0572 (11)	0.0557 (11)	0.0625 (12)	0.0008 (9)	0.0053 (9)	0.0117 (9)
C15	0.0492 (10)	0.0516 (11)	0.0639 (12)	-0.0032 (8)	-0.0011 (8)	-0.0037 (9)
C16	0.0790 (15)	0.108 (2)	0.0574 (13)	-0.0013 (14)	-0.0077 (11)	0.0135 (13)
C17	0.0595 (11)	0.0652 (13)	0.0810 (15)	0.0165 (10)	0.0111 (10)	0.0006 (11)

*Geometric parameters (Å, °)*

S1—C3	1.7664 (19)	C9—H9A	0.9300
S1—C1	1.792 (3)	C10—C15	1.374 (3)
N1—C3	1.249 (2)	C10—C11	1.379 (3)
N1—C4	1.428 (2)	C11—C12	1.381 (3)
N2—C2	1.360 (3)	C11—H11A	0.9300
N2—C3	1.405 (2)	C12—C13	1.383 (3)
N2—C10	1.448 (2)	C12—H12A	0.9300
O1—C2	1.200 (3)	C13—C14	1.385 (3)
C1—C2	1.502 (3)	C13—C16	1.511 (3)
C1—H1A	0.9700	C14—C15	1.381 (3)
C1—H1B	0.9700	C14—H14A	0.9300
C4—C9	1.383 (3)	C15—H15A	0.9300
C4—C5	1.387 (3)	C16—H16A	0.9600

C5—C6	1.387 (3)	C16—H16B	0.9600
C5—H5A	0.9300	C16—H16C	0.9600
C6—C7	1.381 (3)	C17—H17A	0.9600
C6—H6A	0.9300	C17—H17B	0.9600
C7—C8	1.380 (3)	C17—H17C	0.9600
C7—C17	1.511 (3)	C17—H17D	0.9600
C8—C9	1.381 (3)	C17—H17E	0.9600
C8—H8A	0.9300	C17—H17F	0.9600
C3—S1—C1	92.50 (10)	C4—C9—H9A	119.9
C3—N1—C4	119.78 (15)	C15—C10—C11	120.72 (17)
C2—N2—C3	117.32 (15)	C15—C10—N2	119.79 (16)
C2—N2—C10	121.64 (15)	C11—C10—N2	119.46 (17)
C3—N2—C10	120.97 (15)	C10—C11—C12	119.31 (18)
C2—C1—S1	108.16 (17)	C10—C11—H11A	120.3
C2—C1—H1A	110.1	C12—C11—H11A	120.3
S1—C1—H1A	110.1	C11—C12—C13	121.27 (18)
C2—C1—H1B	110.1	C11—C12—H12A	119.4
S1—C1—H1B	110.1	C13—C12—H12A	119.4
H1A—C1—H1B	108.4	C12—C13—C14	118.00 (17)
O1—C2—N2	124.7 (2)	C12—C13—C16	121.1 (2)
O1—C2—C1	123.3 (2)	C14—C13—C16	120.9 (2)
N2—C2—C1	111.96 (18)	C15—C14—C13	121.58 (19)
N1—C3—N2	122.02 (16)	C15—C14—H14A	119.2
N1—C3—S1	127.89 (14)	C13—C14—H14A	119.2
N2—C3—S1	110.05 (13)	C10—C15—C14	119.10 (17)
C9—C4—C5	118.94 (17)	C10—C15—H15A	120.4
C9—C4—N1	118.71 (16)	C14—C15—H15A	120.4
C5—C4—N1	122.16 (17)	C13—C16—H16A	109.5
C6—C5—C4	119.96 (19)	C13—C16—H16B	109.5
C6—C5—H5A	120.0	H16A—C16—H16B	109.5
C4—C5—H5A	120.0	C13—C16—H16C	109.5
C7—C6—C5	121.40 (18)	H16A—C16—H16C	109.5
C7—C6—H6A	119.3	H16B—C16—H16C	109.5
C5—C6—H6A	119.3	C7—C17—H17A	109.5
C8—C7—C6	117.93 (17)	C7—C17—H17B	109.5
C8—C7—C17	120.51 (19)	C7—C17—H17C	109.5
C6—C7—C17	121.51 (19)	C7—C17—H17D	109.5
C7—C8—C9	121.47 (18)	C7—C17—H17E	109.5
C7—C8—H8A	119.3	H17D—C17—H17E	109.5
C9—C8—H8A	119.3	C7—C17—H17F	109.5
C8—C9—C4	120.27 (18)	H17D—C17—H17F	109.5
C8—C9—H9A	119.9	H17E—C17—H17F	109.5
C3—S1—C1—C2	0.6 (3)	C5—C6—C7—C17	-176.1 (2)
C3—N2—C2—O1	178.7 (3)	C6—C7—C8—C9	-2.0 (3)
C10—N2—C2—O1	1.7 (4)	C17—C7—C8—C9	175.62 (19)
C3—N2—C2—C1	-0.4 (3)	C7—C8—C9—C4	1.3 (3)
C10—N2—C2—C1	-177.4 (2)	C5—C4—C9—C8	-0.1 (3)

S1—C1—C2—O1	-179.3 (3)	N1—C4—C9—C8	-175.14 (17)
S1—C1—C2—N2	-0.2 (4)	C2—N2—C10—C15	77.3 (3)
C4—N1—C3—N2	179.14 (16)	C3—N2—C10—C15	-99.6 (2)
C4—N1—C3—S1	1.9 (3)	C2—N2—C10—C11	-101.0 (2)
C2—N2—C3—N1	-176.8 (2)	C3—N2—C10—C11	82.1 (2)
C10—N2—C3—N1	0.2 (3)	C15—C10—C11—C12	0.7 (3)
C2—N2—C3—S1	0.9 (2)	N2—C10—C11—C12	179.01 (17)
C10—N2—C3—S1	177.91 (14)	C10—C11—C12—C13	0.0 (3)
C1—S1—C3—N1	176.7 (2)	C11—C12—C13—C14	-0.5 (3)
C1—S1—C3—N2	-0.82 (19)	C11—C12—C13—C16	179.7 (2)
C3—N1—C4—C9	-118.4 (2)	C12—C13—C14—C15	0.4 (3)
C3—N1—C4—C5	66.7 (3)	C16—C13—C14—C15	-179.9 (2)
C9—C4—C5—C6	-0.4 (3)	C11—C10—C15—C14	-0.9 (3)
N1—C4—C5—C6	174.46 (19)	N2—C10—C15—C14	-179.14 (17)
C4—C5—C6—C7	-0.3 (3)	C13—C14—C15—C10	0.3 (3)
C5—C6—C7—C8	1.5 (3)		

*Hydrogen-bond geometry (Å, °)*

*Cg1* and *Cg2* are the centroids of the S1/N2/C1—C3 and C4—C9 rings, respectively.

<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>
C5—H5 <i>A</i> ... <i>Cg1</i> <sup>i</sup>	0.93	3.00	3.788 (2)	144
C9—H9 <i>A</i> ... <i>Cg2</i> <sup>ii</sup>	0.93	2.87	3.607 (2)	138

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