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Pifithrin-β

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Key indicators

Single-crystal X-ray study
T = 160 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.038
wR factor = 0.103
Data-to-parameter ratio = 16.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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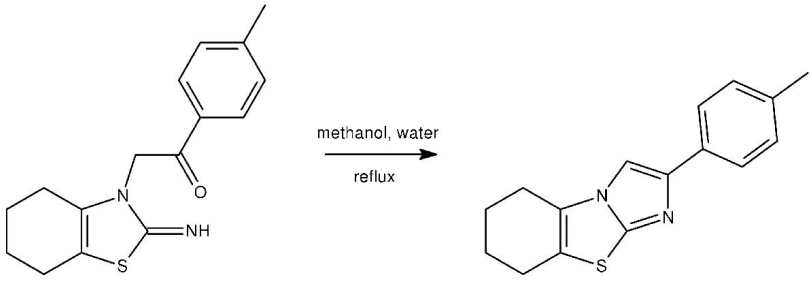
The title compound, 2-*p*-tolyl-5,6,7,8-tetrahydrobenzo[*d*]-imidazo[2,1-*b*]thiazole, $C_{16}H_{16}N_2S$, is a condensation product of pifithrin-α, which has been previously reported as an inhibitor of the tumour suppressor protein p53. The molecule contains a planar fused pair of heterocyclic five-membered rings and the attached *p*-tolyl substituent is also essentially coplanar.

Comment

The compound pifithrin-α [2-(2-imino-4,5,6,7-tetrahydrobenzothiazol-3-yl)-1-(4-methylphenyl)ethanone, (1)] was previously reported to inhibit, *in vitro*, a number of processes involving the tumour suppressor protein p53; it was thus of interest in the development of cancer therapies (Komarov *et al.*, 1999). During a further evaluation of the effectiveness of pifithrin-α, a crystalline sample was obtained and its structure investigated by X-ray diffraction. However, the material was found to be a condensation product of pifithrin-α, from which water had been eliminated in a ring closure. The product, referred to as pifithrin-β, (2), is more stable than pifithrin-α in tissue culture medium. The revelation of this transformation through crystallographic identification of the condensation product has led to an expansion of the original evaluation of pifithrin-α to include also pifithrin-β, and the recognition that some of the inhibitory effects previously ascribed to pifithrin-α are probably due instead to pifithrin-β or a combination of the two compounds (Walton *et al.*, 2005).



(1) (2)

The molecule of pifithrin-β (Fig. 1) contains three fused rings with a *p*-tolyl substituent. The cyclohexene ring (or tetrahydrobenzo group) is disordered over two conformations, in which the two saturated C atoms furthest from the double bond lie one on each side of the mean plane of the other atoms of the ring [by 0.377 (4) and 0.375 (4) Å for the major component]; the two disorder components have opposite senses of twist for this CH_2CH_2 segment (see the torsion angles in Table 1). The fused thiazole and imidazole rings are individually planar (r.m.s. deviations < 0.003 Å) and form a

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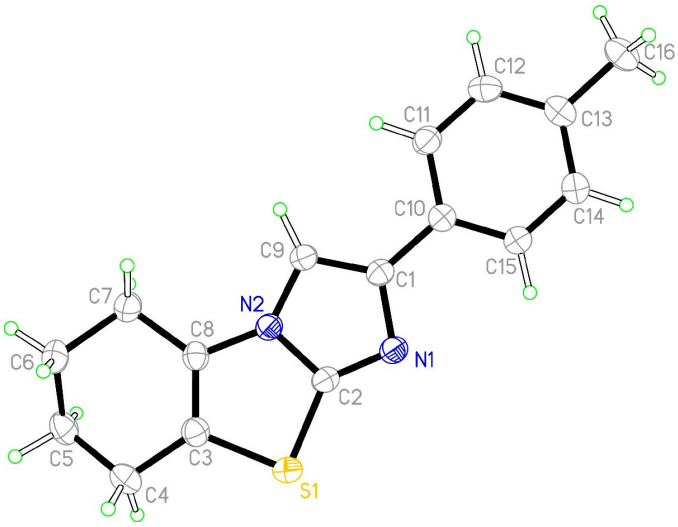

Figure 1
The molecular structure of (2) with atom labels and 50% probability ellipsoids for non-H atoms. The minor disorder component has been omitted.

single planar unit [r.m.s. deviation 0.009 Å; dihedral angle between the two five-membered rings = 1.32 (5)°]. Such imidazo[2,1-*b*]thiazole fused ring systems have been found in ten other crystal structures in the Cambridge Structural Database (Version 5.26 plus one update, February 2005; Allen, 2002), and they are all planar.

The benzene ring of the *p*-tolyl substituent makes a dihedral angle of 2.32 (5)° with the imidazole ring to which it is attached. The whole molecule, excluding H atoms and the disordered CH_2CH_2 linkage, is thus essentially planar, with an r.m.s. deviation of 0.039 Å. There are no notable intermolecular interactions in the crystal structure. The molecules lie in almost planar sheets parallel to (001) (Fig. 2).

Experimental

The compound was prepared by a condensation reaction of pifithrin-α, initially unintentionally during a study of anti-tumour agents, and subsequently by refluxing in aqueous methanol (Walton *et al.*, 2005). It was recrystallized from methanol.

Crystal data

$C_{16}H_{16}N_2S$
M_r = 268.37
Monoclinic, $P2_1/c$
a = 7.1729 (4) Å
b = 13.5386 (8) Å
c = 14.3530 (8) Å
β = 103.917 (2)°
V = 1352.92 (13) Å^3
Z = 4
D_x = 1.318 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9390 reflections
θ = 2.1–28.5°
μ = 0.23 mm^{-1}
T = 160 (2) K
Block, colourless
0.44 × 0.30 × 0.26 mm

Data collection

Bruker SMART 1K CCD diffractometer
Thin-slice ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.91, T_{max} = 0.94
11454 measured reflections
3222 independent reflections
2871 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 28.5°
$h = -9 \rightarrow 9$
$k = -17 \rightarrow 17$
$l = -18 \rightarrow 18$

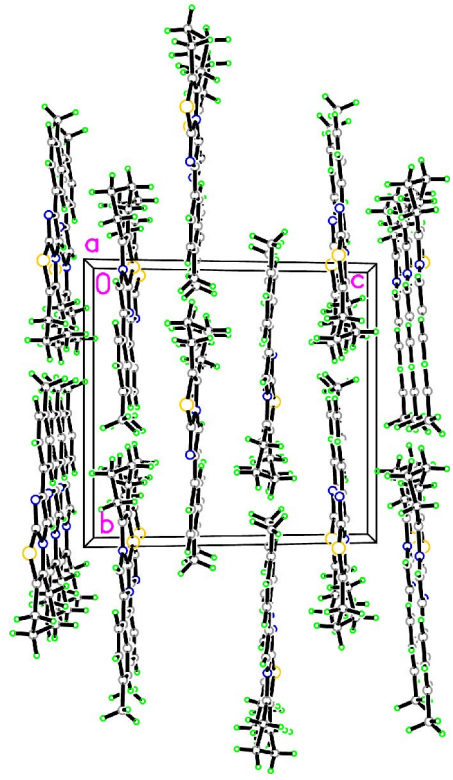

Figure 2
The crystal packing, viewed along the *a* axis, showing almost planar sheets of molecules parallel to (001).

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
S = 1.05
3222 reflections
192 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 0.5147P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.3949 (17)	S1—C2	1.7391 (13)
N1—C2	1.3147 (17)	S1—C3	1.7650 (14)
N2—C2	1.3666 (16)	C1—C9	1.3760 (18)
N2—C8	1.3991 (16)	C3—C8	1.3447 (19)
N2—C9	1.3770 (17)		
C1—N1—C2	103.49 (11)	N1—C2—S1	136.19 (10)
C2—N2—C8	115.28 (11)	N2—C2—S1	110.23 (10)
C2—N2—C9	106.49 (11)	S1—C3—C4	123.59 (10)
C8—N2—C9	138.21 (11)	S1—C3—C8	112.18 (10)
C2—S1—C3	90.36 (6)	C4—C3—C8	124.22 (13)
N1—C1—C9	111.16 (11)	N2—C8—C3	111.96 (11)
N1—C1—C10	121.52 (11)	N2—C8—C7	122.51 (11)
C9—C1—C10	127.32 (12)	C3—C8—C7	125.52 (12)
N1—C2—N2	113.56 (11)	N2—C9—C1	105.31 (11)
C3—C4—C5—C6	−45.8 (3)	C5*X*—C6*X*—C7—C8	41.1 (9)
C4—C5—C6—C7	64.3 (3)	C5—C6—C7—C8	−45.5 (3)
C3—C4—C5*X*—C6*X*	47.9 (8)	N1—C1—C10—C15	−1.16 (19)
C4—C5*X*—C6*X*—C7	−61.1 (10)	C9—C1—C10—C11	−1.5 (2)

H atoms were positioned geometrically (C—H = 0.95–0.99 Å) and refined with a riding model (including free rotation about the C—C bond for the methyl group), and with U_{iso} values constrained to be 1.2

(1.5 for methyl groups) times U_{eq} of the carrier atom. Twofold disorder was resolved and refined for the central CH_2CH_2 linkage of the cyclohexene ring, with occupancy factors 0.766 (6):0.234 (6).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Komarov, P. G., Komarova, E. A., Kondratov, R. V, Christov-Tselkov, K., Coon, J. S., Chernov, M. V. & Gudkov, A. V. (1999). *Science*, **285**, 1733–1737.
Sheldrick, G. M. (2001). *SHELXTL*. Version 6. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
Walton, M. I., Wilson, S. C., Hardcastle, I. R., Mirza, A. R. & Workman, P. (2005). *Mol. Cancer Ther.* In the press.

supporting information

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$F(000) = 568$
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Cell parameters from 9390 reflections
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Graphite monochromator
Detector resolution: 8.192 pixels mm^{-1}
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$R_{int} = 0.022$
$\theta_{max} = 28.5°$, $\theta_{min} = 2.1°$
$h = -9 \rightarrow 9$
$k = -17 \rightarrow 17$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.103$
$S = 1.05$
3222 reflections
192 parameters
36 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
$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 0.5147P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1	0.58299 (16)	0.17620 (8)	0.14058 (8)	0.0257 (2)	
N2	0.69620 (16)	0.02495 (8)	0.12171 (8)	0.0242 (2)	
S1	0.35910 (5)	0.00517 (3)	0.14928 (3)	0.03065 (12)	

C1	0.76869 (18)	0.18220 (10)	0.12686 (9)	0.0237 (3)	
C2	0.54752 (18)	0.08082 (10)	0.13678 (9)	0.0242 (3)	
C3	0.4914 (2)	−0.10047 (10)	0.13244 (9)	0.0268 (3)	
C4	0.4184 (2)	−0.20417 (11)	0.13456 (11)	0.0326 (3)	
H4A	0.3239	−0.2189	0.0736	0.039*	0.766 (6)
H4B	0.3535	−0.2114	0.1877	0.039*	0.766 (6)
H4X	0.2834	−0.2088	0.0971	0.039*	0.234 (6)
H4Y	0.4246	−0.2247	0.2014	0.039*	0.234 (6)
C5	0.5846 (3)	−0.27551 (14)	0.1484 (2)	0.0333 (6)	0.766 (6)
H5A	0.5345	−0.3435	0.1347	0.040*	0.766 (6)
H5B	0.6590	−0.2732	0.2161	0.040*	0.766 (6)
C6	0.7167 (4)	−0.25056 (15)	0.0826 (2)	0.0316 (6)	0.766 (6)
H6A	0.6409	−0.2503	0.0152	0.038*	0.766 (6)
H6B	0.8164	−0.3023	0.0890	0.038*	0.766 (6)
C5X	0.5584 (10)	−0.2755 (5)	0.0866 (7)	0.035 (2)	0.234 (6)
H5X1	0.5311	−0.3456	0.0980	0.042*	0.234 (6)
H5X2	0.5273	−0.2647	0.0163	0.042*	0.234 (6)
C6X	0.7701 (13)	−0.2555 (6)	0.1274 (8)	0.0367 (19)	0.234 (6)
H6X1	0.8478	−0.3011	0.0981	0.044*	0.234 (6)
H6X2	0.8033	−0.2670	0.1976	0.044*	0.234 (6)
C7	0.8147 (2)	−0.14939 (10)	0.10651 (11)	0.0304 (3)	
H7A	0.9181	−0.1539	0.1661	0.036*	0.766 (6)
H7B	0.8721	−0.1278	0.0537	0.036*	0.766 (6)
H7X	0.9395	−0.1306	0.1494	0.036*	0.234 (6)
H7Y	0.8282	−0.1451	0.0396	0.036*	0.234 (6)
C8	0.66567 (19)	−0.07719 (9)	0.11945 (9)	0.0249 (3)	
C9	0.84012 (19)	0.08993 (10)	0.11508 (10)	0.0258 (3)	
H9	0.9626	0.0744	0.1046	0.031*	
C10	0.86652 (18)	0.27755 (10)	0.12710 (9)	0.0241 (3)	
C11	1.05548 (19)	0.28174 (10)	0.11660 (10)	0.0291 (3)	
H11	1.1197	0.2224	0.1077	0.035*	
C12	1.1500 (2)	0.37143 (11)	0.11911 (10)	0.0315 (3)	
H12	1.2785	0.3722	0.1122	0.038*	
C13	1.0616 (2)	0.46007 (10)	0.13146 (9)	0.0288 (3)	
C14	0.8730 (2)	0.45609 (11)	0.14183 (10)	0.0317 (3)	
H14	0.8092	0.5156	0.1507	0.038*	
C15	0.7773 (2)	0.36671 (10)	0.13934 (10)	0.0294 (3)	
H15	0.6487	0.3661	0.1461	0.035*	
C16	1.1659 (2)	0.55676 (11)	0.13264 (11)	0.0360 (3)	
H16A	1.3047	0.5455	0.1534	0.054*	
H16B	1.1261	0.6024	0.1772	0.054*	
H16C	1.1348	0.5854	0.0680	0.054*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0233 (5)	0.0267 (5)	0.0276 (5)	0.0019 (4)	0.0071 (4)	0.0006 (4)
N2	0.0238 (5)	0.0234 (5)	0.0262 (5)	0.0018 (4)	0.0080 (4)	0.0015 (4)

S1	0.02331 (18)	0.02947 (19)	0.0411 (2)	−0.00072 (12)	0.01156 (14)	0.00096 (14)
C1	0.0233 (6)	0.0262 (6)	0.0220 (6)	0.0019 (5)	0.0060 (5)	0.0012 (5)
C2	0.0214 (6)	0.0265 (6)	0.0253 (6)	0.0021 (5)	0.0069 (5)	0.0010 (5)
C3	0.0279 (6)	0.0256 (6)	0.0266 (6)	0.0007 (5)	0.0059 (5)	0.0017 (5)
C4	0.0337 (7)	0.0292 (7)	0.0348 (7)	−0.0068 (6)	0.0081 (6)	0.0019 (6)
C5	0.0387 (11)	0.0231 (9)	0.0372 (16)	−0.0024 (7)	0.0074 (9)	0.0046 (8)
C6	0.0373 (13)	0.0232 (9)	0.0350 (14)	0.0043 (8)	0.0098 (10)	−0.0003 (10)
C5X	0.039 (4)	0.026 (3)	0.037 (5)	0.000 (2)	0.005 (3)	0.003 (3)
C6X	0.042 (4)	0.031 (3)	0.032 (4)	0.000 (3)	0.000 (3)	−0.001 (3)
C7	0.0314 (7)	0.0255 (6)	0.0358 (7)	0.0029 (5)	0.0114 (6)	0.0013 (5)
C8	0.0285 (6)	0.0219 (6)	0.0244 (6)	0.0011 (5)	0.0064 (5)	0.0018 (5)
C9	0.0236 (6)	0.0249 (6)	0.0305 (6)	0.0013 (5)	0.0094 (5)	0.0019 (5)
C10	0.0250 (6)	0.0254 (6)	0.0215 (6)	0.0003 (5)	0.0048 (5)	0.0007 (5)
C11	0.0268 (7)	0.0293 (7)	0.0320 (7)	0.0014 (5)	0.0083 (5)	−0.0032 (5)
C12	0.0249 (6)	0.0383 (8)	0.0319 (7)	−0.0043 (5)	0.0079 (5)	−0.0028 (6)
C13	0.0323 (7)	0.0305 (7)	0.0219 (6)	−0.0070 (5)	0.0033 (5)	−0.0005 (5)
C14	0.0337 (7)	0.0254 (7)	0.0368 (7)	0.0010 (5)	0.0101 (6)	0.0012 (5)
C15	0.0261 (7)	0.0270 (6)	0.0366 (7)	0.0014 (5)	0.0101 (5)	0.0017 (5)
C16	0.0391 (8)	0.0340 (7)	0.0332 (7)	−0.0118 (6)	0.0053 (6)	−0.0003 (6)

Geometric parameters (Å, º)

N1—C1	1.3949 (17)	C5X—C6X	1.515 (12)
N1—C2	1.3147 (17)	C6X—H6X1	0.990
N2—C2	1.3666 (16)	C6X—H6X2	0.990
N2—C8	1.3991 (16)	C6X—C7	1.518 (8)
N2—C9	1.3770 (17)	C7—H7A	0.990
S1—C2	1.7391 (13)	C7—H7B	0.990
S1—C3	1.7650 (14)	C7—H7X	0.990
C1—C9	1.3760 (18)	C7—H7Y	0.990
C1—C10	1.4689 (18)	C7—C8	1.4926 (18)
C3—C4	1.5014 (19)	C9—H9	0.950
C3—C8	1.3447 (19)	C10—C11	1.4005 (18)
C4—H4A	0.990	C10—C15	1.3971 (18)
C4—H4B	0.990	C11—H11	0.950
C4—H4X	0.990	C11—C12	1.387 (2)
C4—H4Y	0.990	C12—H12	0.950
C4—C5	1.510 (2)	C12—C13	1.389 (2)
C4—C5X	1.658 (7)	C13—C14	1.397 (2)
C5—H5A	0.990	C13—C16	1.5061 (19)
C5—H5B	0.990	C14—H14	0.950
C5—C6	1.528 (3)	C14—C15	1.388 (2)
C6—H6A	0.990	C15—H15	0.950
C6—H6B	0.990	C16—H16A	0.980
C6—C7	1.540 (3)	C16—H16B	0.980
C5X—H5X1	0.990	C16—H16C	0.980
C5X—H5X2	0.990		

C1—N1—C2	103.49 (11)	C5X—C6X—C7	109.4 (7)
C2—N2—C8	115.28 (11)	H6X1—C6X—H6X2	108.2
C2—N2—C9	106.49 (11)	H6X1—C6X—C7	109.8
C8—N2—C9	138.21 (11)	H6X2—C6X—C7	109.8
C2—S1—C3	90.36 (6)	C6—C7—H7A	110.1
N1—C1—C9	111.16 (11)	C6—C7—H7B	110.1
N1—C1—C10	121.52 (11)	C6—C7—C8	107.94 (13)
C9—C1—C10	127.32 (12)	C6X—C7—H7X	108.8
N1—C2—N2	113.56 (11)	C6X—C7—H7Y	108.8
N1—C2—S1	136.19 (10)	C6X—C7—C8	113.9 (3)
N2—C2—S1	110.23 (10)	H7A—C7—H7B	108.4
S1—C3—C4	123.59 (10)	H7A—C7—C8	110.1
S1—C3—C8	112.18 (10)	H7B—C7—C8	110.1
C4—C3—C8	124.22 (13)	H7X—C7—H7Y	107.7
C3—C4—H4A	109.8	H7X—C7—C8	108.8
C3—C4—H4B	109.8	H7Y—C7—C8	108.8
C3—C4—H4X	110.4	N2—C8—C3	111.96 (11)
C3—C4—H4Y	110.4	N2—C8—C7	122.51 (11)
C3—C4—C5	109.43 (13)	C3—C8—C7	125.52 (12)
C3—C4—C5X	106.7 (2)	N2—C9—C1	105.31 (11)
H4A—C4—H4B	108.2	N2—C9—H9	127.3
H4A—C4—C5	109.8	C1—C9—H9	127.3
H4B—C4—C5	109.8	C1—C10—C11	120.64 (12)
H4X—C4—H4Y	108.6	C1—C10—C15	121.77 (12)
H4X—C4—C5X	110.4	C11—C10—C15	117.59 (12)
H4Y—C4—C5X	110.4	C10—C11—H11	119.6
C4—C5—H5A	109.4	C10—C11—C12	120.84 (13)
C4—C5—H5B	109.4	H11—C11—C12	119.6
C4—C5—C6	111.4 (2)	C11—C12—H12	119.2
H5A—C5—H5B	108.0	C11—C12—C13	121.61 (13)
H5A—C5—C6	109.4	H12—C12—C13	119.2
H5B—C5—C6	109.4	C12—C13—C14	117.66 (13)
C5—C6—H6A	109.2	C12—C13—C16	120.75 (14)
C5—C6—H6B	109.2	C14—C13—C16	121.58 (14)
C5—C6—C7	112.1 (2)	C13—C14—H14	119.4
H6A—C6—H6B	107.9	C13—C14—C15	121.12 (13)
H6A—C6—C7	109.2	H14—C14—C15	119.4
H6B—C6—C7	109.2	C10—C15—C14	121.18 (13)
C4—C5X—H5X1	109.0	C10—C15—H15	119.4
C4—C5X—H5X2	109.0	C14—C15—H15	119.4
C4—C5X—C6X	112.7 (6)	C13—C16—H16A	109.5
H5X1—C5X—H5X2	107.8	C13—C16—H16B	109.5
H5X1—C5X—C6X	109.0	C13—C16—H16C	109.5
H5X2—C5X—C6X	109.0	H16A—C16—H16B	109.5
C5X—C6X—H6X1	109.8	H16A—C16—H16C	109.5
C5X—C6X—H6X2	109.8	H16B—C16—H16C	109.5

C2—N1—C1—C9	0.04 (14)	C2—N2—C8—C3	0.29 (16)

C2—N1—C1—C10	−179.28 (11)	C2—N2—C8—C7	−178.23 (12)
C1—N1—C2—N2	0.03 (14)	C9—N2—C8—C3	178.36 (15)
C1—N1—C2—S1	177.90 (12)	C9—N2—C8—C7	−0.2 (2)
C8—N2—C2—N1	178.58 (11)	C6—C7—C8—N2	−166.19 (16)
C8—N2—C2—S1	0.15 (14)	C6—C7—C8—C3	15.5 (2)
C9—N2—C2—N1	−0.08 (15)	C6X—C7—C8—N2	167.5 (5)
C9—N2—C2—S1	−178.51 (9)	C6X—C7—C8—C3	−10.8 (5)
C3—S1—C2—N1	−178.32 (15)	N1—C1—C9—N2	−0.08 (15)
C3—S1—C2—N2	−0.39 (10)	C10—C1—C9—N2	179.18 (12)
C2—S1—C3—C4	179.36 (12)	C2—N2—C9—C1	0.10 (14)
C2—S1—C3—C8	0.57 (11)	C8—N2—C9—C1	−178.09 (14)
S1—C3—C4—C5	−162.66 (15)	N1—C1—C10—C11	177.71 (12)
S1—C3—C4—C5X	164.7 (3)	N1—C1—C10—C15	−1.16 (19)
C8—C3—C4—C5	16.0 (2)	C9—C1—C10—C11	−1.5 (2)
C8—C3—C4—C5X	−16.7 (4)	C9—C1—C10—C15	179.65 (13)
C3—C4—C5—C6	−45.8 (3)	C1—C10—C11—C12	−178.43 (12)
C4—C5—C6—C7	64.3 (3)	C15—C10—C11—C12	0.5 (2)
C3—C4—C5X—C6X	47.9 (8)	C10—C11—C12—C13	−0.4 (2)
C4—C5X—C6X—C7	−61.1 (10)	C11—C12—C13—C14	0.3 (2)
C5X—C6X—C7—C8	41.1 (9)	C11—C12—C13—C16	−179.17 (13)
C5—C6—C7—C8	−45.5 (3)	C12—C13—C14—C15	−0.3 (2)
S1—C3—C8—N2	−0.59 (14)	C16—C13—C14—C15	179.12 (13)
S1—C3—C8—C7	177.88 (11)	C13—C14—C15—C10	0.5 (2)
C4—C3—C8—N2	−179.37 (12)	C1—C10—C15—C14	178.36 (13)
C4—C3—C8—C7	−0.9 (2)	C11—C10—C15—C14	−0.5 (2)