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4-[(*tert*-Butyldiphenylsilyloxy)methyl]-pyridazin-3(2*H*)-one

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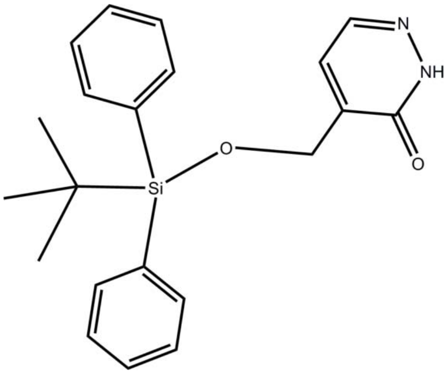
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.046; wR factor = 0.148; data-to-parameter ratio = 20.8.

In the title compound, $C_{21}H_{24}N_2O_2Si$, the carbonyl group of the heterocyclic ring and the O atom of the silyl ether group are placed toward opposite sides and the *tert*-butyl and pyridazinone moieties are *anti*-oriented across the Si—O bond [torsion angle = −168.44 (19)°]. In the crystal, molecules are assembled into inversion dimers through co-operative N—H···O hydrogen bonds between the NH groups and O atoms of the pyridazinone rings of neighbouring molecules. The dimers are linked by π–π interactions involving adjacent pyridazinone rings [centroid–centroid distance = 3.8095 (19) Å], generating ladder-like chains along the b-axis direction. The chains are further linked into a two-dimensional network parallel to the ab plane through weak C—H···π interactions.

Related literature

For background to pyridazinone analogues displaying biological activities, see: Siddiqui *et al.* (2010); Costas *et al.* (2010); Abouzid & Bekhit (2008); Cesari *et al.* (2006); Rathish *et al.* (2009); Al-Tel (2010); Suree *et al.* (2009); Tao *et al.* (2011). For related structures, see: Costas *et al.* (2010); Costas-Lago *et al.* (2013).



Experimental

Crystal data

$C_{21}H_{24}N_2O_2Si$
M_r = 364.51
Monoclinic, $P2_1/n$
a = 10.774 (4) Å
b = 7.988 (3) Å
c = 24.681 (10) Å
β = 100.207 (7)°
V = 2090.5 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 293 K
0.48 × 0.41 × 0.23 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.707, $T_{\max}$ = 0.746
25187 measured reflections
5045 independent reflections
3076 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.148
S = 1.00
5045 reflections
242 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$ = 0.30 e Å^{-3}
$\Delta\rho_{\min}$ = −0.24 e Å^{-3}

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

*Cg*2 is the centroid of the C8′–C13′ ring

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3^{i}	0.93 (3)	1.84 (3)	2.764 (2)	176 (2)
C6—H6···$Cg2^{ii}$	0.93	2.76	3.637 (3)	138

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LR2118).

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o1860 Costas-Lago *et al.* • $C_{21}H_{24}N_2O_2Si$ *Acta Cryst.* (2013). E**69**, o1859–o1860

supporting information

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4-[(*tert*-Butyldiphenylsilyloxy)methyl]pyridazin-3(2*H*)-one

María Carmen Costas-Lago, Tamara Costas, Noemí Vila and Pedro Besada

S1. Introduction

Pyridazin-3(2*H*)-one derivatives possess a wide range of biological activities, this fact together with the easy functionalization at various ring positions makes the pyridazinone nucleus a versatile pharmacophore to design and synthesize new drugs. For instance, an important number of pyridazinones have been reported as antihypertensive (Siddiqui *et al.*, 2010), antiplatelet (Costas *et al.*, 2010), anti-inflammatory (Abouzid & Bekhit, 2008), antinociceptive (Cesari *et al.*, 2006), antidiabetic (Rathish *et al.*, 2009), anticancer (Al-Tel, 2010), antimicrobial (Suree *et al.*, 2009) or anti-histamine H_3 agents (Tao *et al.*, 2011).

S2. Experimental

S2.1. Synthesis and crystallization

A solution of 3-(*tert*-butyldiphenylsilyloxymethyl)-5-hydroxy-5*H*-furan-2-ona (50 mg, 0.136 mmol) and hydrazine monohydrate (14 ml, 0.284 mmol) in ethanol (2 ml) was stirred at reflux for 4 h. The solvent was evaporated under reduced pressure and residue was purified by column chromatography on silica gel (hexane/ethyl acetate 4:1) to afford a colourless oil (16 mg, 32%). Single crystals suitable for X-ray analysis were grown from a chloroform solution at room temperature.

S2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All H-atoms were positioned and refined using a riding model with d(C—H)= 0.93 Å, $U_{iso} = 1.2U_{eq}(C)$ for aromatic C—H groups,d(C—H)= 0.97 Å, $U_{iso} = 1.2U_{eq}(C)$ for CH_2 group and d(C—H)= 0.96 Å, $U_{iso} = 1.5U_{eq}(C)$ for CH_3 group; except for the hydrogen atoms of the NH group which were located from a Fourier-difference map and refined isotropically

S3. Results and discussion

The compound I, an isomer of the 5-(*tert*-butyldiphenylsilyloxymethyl)pyridazin-3(2*H*)-one (Costas-Lago *et al.*, 2013), was prepared in order to develop new pyridazinone analogues C4-substituted as antiplatelet agents. In the titled compound, the carbonyl group of the heterocyclic ring and the oxygen atom of the silyl ether group are placed toward opposite sides, this contrasts with the geometry found in the C5-substituted regioisomer and could explain the nearly flat disposition of the sequence C4—C1′-O1′-Si, with a torsion angle of -174.30 (15)°. The pyridazinone ring forms dihedral angles of 89.10 (8)° and 77.53 (7)°, respectively, with the C2′-C7′ and C8′-C13′ benzene rings, while the dihedral angle between both benzene rings is 48.41 (10)°.

The geometry of titled compound lets the assembly of molecules in supramolecular organizations based on hydrogen bonding, π–π and CH···π interactions. The cooperative N—H···O hydrogen bonds between the NH group of one pyridazinone ring and the oxygen atom of an adjacent ring form supramolecular dimers (Figure 2). These dimers are joined by π–π interactions involving also neighbouring pyridazinone rings [*Cg*(1): N1—N2—C3—C4—C5—C6; d[*Cg*(1)—*Cg*(1)^{ii}]: 3.8095 (19) Å; d[*Cg*(1)···P(1)^{ii}]: 3.4279 (8) Å; α: 0°; symmetry code ii: 1 - *x*, 2 - *y*, -*z*] resulting in a ladder chain along the crystallographic *b* axis (Figure 3). Finally, the linear chains are linked into a two-dimensional network through weak C—H···π interactions (Figure 4) involving CH groups of the pyridazinone rings and phenyl rings from neighbouring chains [C6—H6···*Cg*(2)^{iii}; *Cg*(2): C8′-C9′-C10′-C11′-C12′-C13′; d[H···*Cg*(2)^{iii}]: 2.890 Å; γ: 17.60°; symmetry code iii: 2 - *x*, -2 - *y*, -*z*]. In this case the pyridazinone ring arrangement prevents the three-dimensional growth observed in the C5-substituted regioisomer (Costas-Lago *et al.*, 2013).

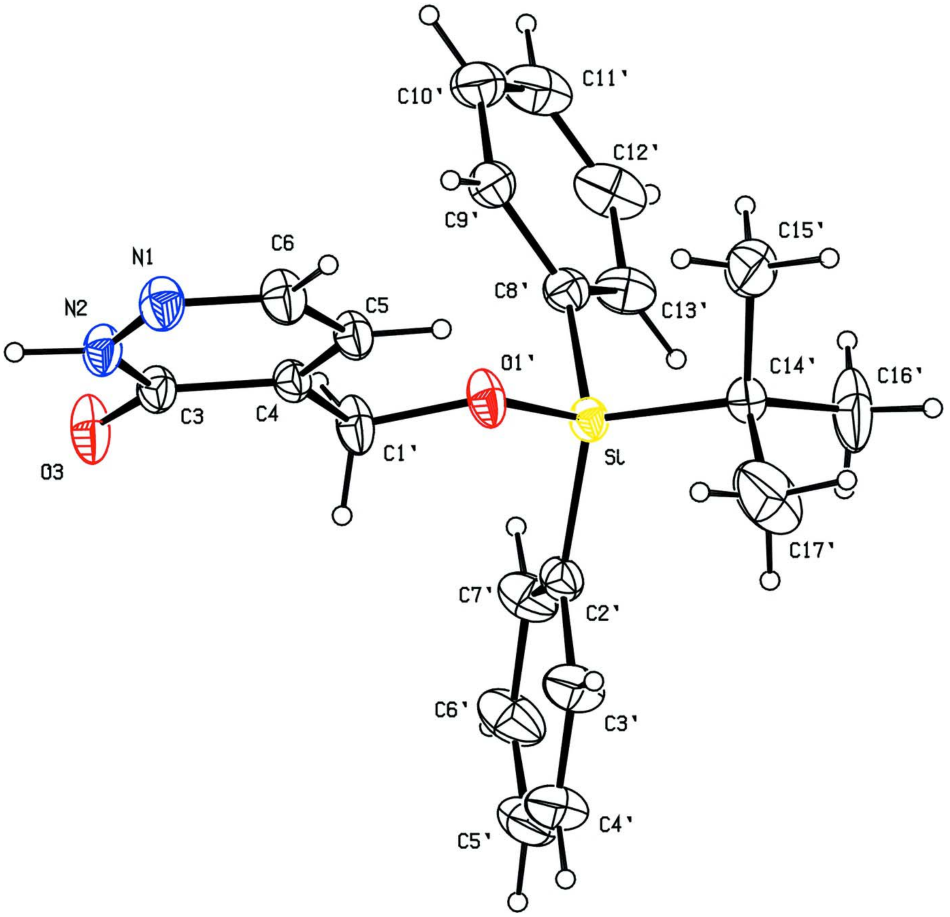

Figure 1

The molecular structure of (I) showing the atom-numbering scheme. Displacement ellipsoids are shown at the 20% probability level.

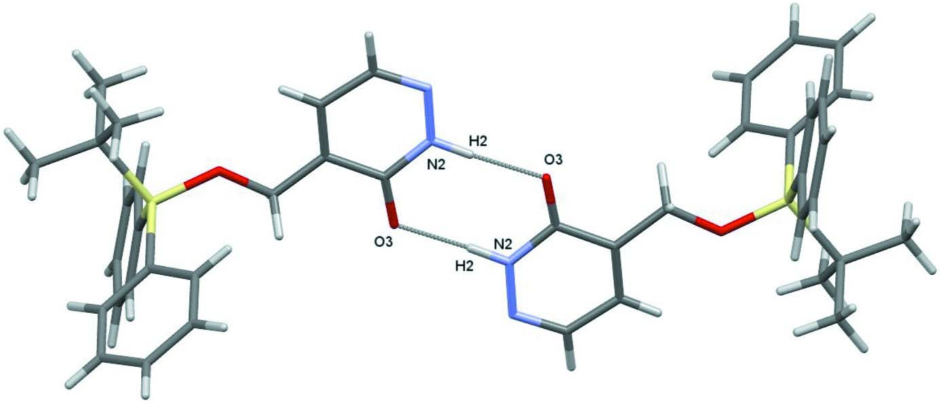

Figure 2

View of supramolecular dimer generated by NH···O hydrogen bonds.

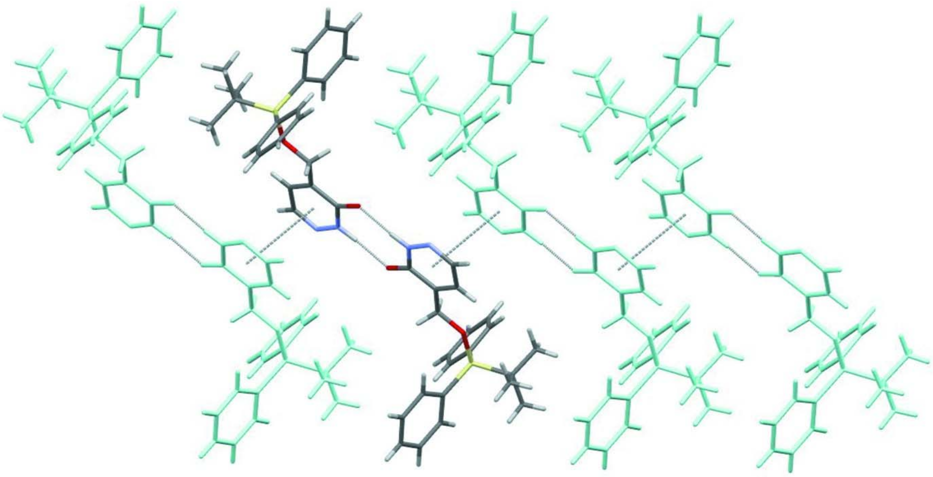

Figure 3

View of the ladder chain along crystallographic *b* axis generated by π–π interactions.

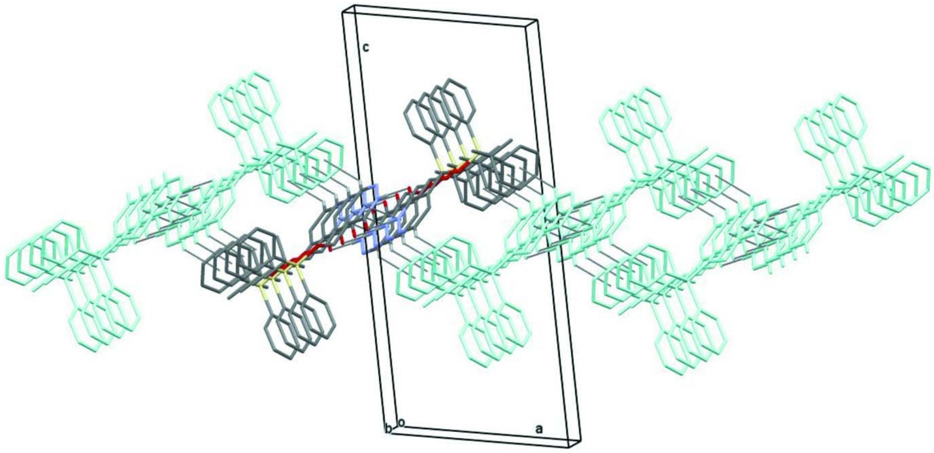

Figure 4

View of the two-dimensional organization generated by CH···π interactions (H atoms, no-involved in supramolecular structure, have been omitted to clarify).

4-[(*tert*-Butyldiphenylsilyloxy)methyl]pyridazin-3(2*H*)-one

Crystal data

$C_{21}H_{24}N_2O_2Si$	$F(000) = 776$
$M_r = 364.51$	$D_x = 1.158$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 5037 reflections
$a = 10.774$ (4) Å	$\theta = 2.7$–23.0°
$b = 7.988$ (3) Å	$\mu = 0.13$ mm^{-1}
$c = 24.681$ (10) Å	$T = 293$ K
$\beta = 100.207$ (7)°	Prism, colourless
$V = 2090.5$ (14) Å^3	0.48 × 0.41 × 0.23 mm
$Z = 4$	

Data collection

Bruker SMART 1000 CCD diffractometer	25187 measured reflections
Radiation source: fine-focus sealed tube	5045 independent reflections
Graphite monochromator	3076 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\rm int} = 0.038$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{\rm max} = 28.0°$, $\theta_{\rm min} = 1.7°$
$T_{\rm min} = 0.707$, $T_{\rm max} = 0.746$	$h = -14 \rightarrow 14$
	$k = -10 \rightarrow 10$
	$l = -32 \rightarrow 32$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.148$	$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2 + 0.7126P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\rm max} < 0.001$
5045 reflections	$\Delta\rho_{\rm max} = 0.30$ e Å^{-3}
242 parameters	$\Delta\rho_{\rm min} = -0.24$ e Å^{-3}
0 restraints	
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. ^{1}H-RMN (400 MHz, CDCl$_3$) δ p.p.m.: 12.32 (s, 1H), 7.90 (d, 1H, J=4.0 Hz), 7.65 (m, 4H), 7.60 (m, 1H), 7.42 (m, 6H), 4.77 (d, 2H, J=1.7 Hz), 1.14 (s, 9H).

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	$U_{\rm iso}$*/$U_{\rm eq}$
Si	0.99974 (5)	0.99175 (7)	0.14301 (2)	0.04561 (17)
N1	0.52674 (18)	0.8319 (2)	−0.06086 (7)	0.0653 (5)

H2	0.487 (2)	0.611 (4)	−0.0346 (11)	0.086 (8)*
N2	0.53846 (17)	0.7036 (2)	−0.02487 (7)	0.0574 (5)
C3	0.62195 (19)	0.6898 (3)	0.02344 (8)	0.0526 (5)
O3	0.62352 (16)	0.5633 (2)	0.05259 (7)	0.0788 (5)
C4	0.70446 (17)	0.8303 (2)	0.03690 (8)	0.0467 (4)
C5	0.6944 (2)	0.9595 (3)	0.00182 (8)	0.0560 (5)
H5	0.7469	1.0521	0.0097	0.067*
C6	0.6037 (2)	0.9546 (3)	−0.04720 (9)	0.0669 (6)
H6	0.5993	1.0454	−0.0710	0.080*
C1′	0.7958 (2)	0.8211 (3)	0.08991 (9)	0.0653 (6)
H1′1	0.7505	0.8207	0.1206	0.078*
H1′2	0.8444	0.7185	0.0913	0.078*
O1′	0.87743 (14)	0.96100 (19)	0.09397 (6)	0.0627 (4)
C2′	0.95347 (19)	0.9463 (3)	0.21122 (8)	0.0543 (5)
C3′	0.8587 (3)	1.0372 (4)	0.22883 (12)	0.0840 (8)
H3′	0.8172	1.1198	0.2059	0.101*
C4′	0.8235 (3)	1.0095 (5)	0.27923 (15)	0.1019 (11)
H4′	0.7594	1.0733	0.2897	0.122*
C5′	0.8812 (3)	0.8910 (5)	0.31327 (12)	0.0971 (11)
H5′	0.8589	0.8741	0.3476	0.117*
C6′	0.9719 (3)	0.7968 (5)	0.29721 (11)	0.0973 (10)
H6′	1.0109	0.7131	0.3203	0.117*
C7′	1.0078 (2)	0.8232 (4)	0.24653 (10)	0.0762 (7)
H7′	1.0702	0.7559	0.2363	0.091*
C8′	1.1303 (2)	0.8497 (3)	0.13054 (8)	0.0552 (5)
C9′	1.1229 (3)	0.7655 (3)	0.08041 (10)	0.0686 (6)
H9′	1.0508	0.7771	0.0537	0.082*
C10′	1.2208 (3)	0.6650 (3)	0.06949 (14)	0.0907 (9)
H10′	1.2141	0.6115	0.0356	0.109*
C11′	1.3262 (4)	0.6449 (4)	0.10820 (17)	0.1030 (11)
H11′	1.3910	0.5763	0.1009	0.124*
C12′	1.3376 (3)	0.7244 (4)	0.15767 (15)	0.0950 (10)
H12′	1.4101	0.7105	0.1840	0.114*
C13′	1.2403 (2)	0.8268 (3)	0.16862 (10)	0.0727 (7)
H13′	1.2492	0.8813	0.2024	0.087*
C14′	1.0445 (2)	1.2154 (3)	0.13265 (9)	0.0551 (5)
C15′	1.0735 (3)	1.2322 (4)	0.07485 (11)	0.1004 (10)
H15A	1.0925	1.3469	0.0681	0.151*
H15B	1.0016	1.1971	0.0486	0.151*
H15C	1.1446	1.1633	0.0714	0.151*
C16′	1.1613 (3)	1.2610 (4)	0.17343 (14)	0.1250 (14)
H16A	1.1790	1.3780	0.1702	0.188*
H16B	1.2314	1.1963	0.1659	0.188*
H16C	1.1477	1.2377	0.2101	0.188*
C17′	0.9393 (4)	1.3371 (4)	0.1387 (2)	0.1496 (19)
H17A	0.9230	1.3325	0.1756	0.224*
H17B	0.8643	1.3072	0.1134	0.224*
H17C	0.9643	1.4486	0.1308	0.224*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si	0.0432 (3)	0.0493 (3)	0.0416 (3)	−0.0068 (2)	0.0000 (2)	0.0014 (2)
N1	0.0713 (12)	0.0678 (12)	0.0512 (10)	−0.0148 (10)	−0.0044 (9)	0.0040 (9)
N2	0.0613 (11)	0.0557 (11)	0.0497 (10)	−0.0158 (9)	−0.0052 (8)	−0.0022 (8)
C3	0.0539 (12)	0.0536 (12)	0.0476 (11)	−0.0110 (9)	0.0012 (9)	−0.0008 (9)
O3	0.0872 (12)	0.0635 (10)	0.0720 (10)	−0.0326 (9)	−0.0229 (9)	0.0162 (8)
C4	0.0433 (10)	0.0514 (11)	0.0443 (10)	−0.0101 (8)	0.0048 (8)	−0.0012 (8)
C5	0.0542 (12)	0.0579 (12)	0.0537 (12)	−0.0164 (10)	0.0032 (9)	0.0023 (10)
C6	0.0732 (15)	0.0685 (15)	0.0541 (12)	−0.0161 (12)	−0.0021 (11)	0.0137 (11)
C1′	0.0649 (14)	0.0621 (14)	0.0607 (13)	−0.0267 (11)	−0.0119 (11)	0.0113 (11)
O1′	0.0576 (9)	0.0637 (9)	0.0584 (8)	−0.0250 (7)	−0.0126 (7)	0.0132 (7)
C2′	0.0464 (11)	0.0659 (13)	0.0495 (11)	−0.0099 (10)	0.0057 (9)	0.0012 (10)
C3′	0.0783 (17)	0.093 (2)	0.0888 (19)	0.0090 (15)	0.0360 (15)	0.0102 (15)
C4′	0.091 (2)	0.129 (3)	0.098 (2)	−0.010 (2)	0.0526 (19)	−0.014 (2)
C5′	0.0764 (19)	0.160 (3)	0.0581 (16)	−0.042 (2)	0.0211 (14)	−0.0041 (19)
C6′	0.0731 (17)	0.153 (3)	0.0643 (16)	−0.0122 (19)	0.0081 (14)	0.0392 (18)
C7′	0.0620 (14)	0.103 (2)	0.0648 (14)	0.0018 (14)	0.0150 (12)	0.0238 (14)
C8′	0.0649 (13)	0.0515 (12)	0.0507 (11)	0.0008 (10)	0.0140 (10)	0.0082 (9)
C9′	0.0959 (18)	0.0508 (13)	0.0650 (14)	−0.0103 (12)	0.0308 (13)	0.0029 (11)
C10′	0.140 (3)	0.0508 (14)	0.099 (2)	−0.0047 (17)	0.070 (2)	0.0005 (14)
C11′	0.126 (3)	0.0723 (19)	0.130 (3)	0.0320 (19)	0.077 (2)	0.034 (2)
C12′	0.0816 (19)	0.105 (2)	0.105 (2)	0.0336 (17)	0.0335 (17)	0.0447 (19)
C13′	0.0700 (15)	0.0858 (18)	0.0648 (14)	0.0173 (13)	0.0189 (12)	0.0162 (13)
C14′	0.0545 (12)	0.0520 (12)	0.0589 (12)	−0.0104 (10)	0.0100 (10)	−0.0043 (10)
C15′	0.164 (3)	0.0717 (18)	0.0710 (17)	−0.0341 (19)	0.0367 (19)	0.0069 (14)
C16′	0.146 (3)	0.107 (3)	0.103 (2)	−0.080 (2)	−0.030 (2)	0.0063 (19)
C17′	0.137 (3)	0.0609 (19)	0.278 (6)	0.0174 (19)	0.109 (4)	0.031 (3)

Geometric parameters (Å, º)

Si—O1′	1.6420 (15)	C6′—C7′	1.390 (4)
Si—C2′	1.874 (2)	C6′—H6′	0.9300
Si—C8′	1.874 (2)	C7′—H7′	0.9300
Si—C14′	1.880 (2)	C8′—C13′	1.388 (3)
N1—C6	1.290 (3)	C8′—C9′	1.398 (3)
N1—N2	1.347 (3)	C9′—C10′	1.389 (4)
N2—C3	1.365 (3)	C9′—H9′	0.9300
N2—H2	0.93 (3)	C10′—C11′	1.358 (5)
C3—O3	1.239 (2)	C10′—H10′	0.9300
C3—C4	1.433 (3)	C11′—C12′	1.363 (5)
C4—C5	1.340 (3)	C11′—H11′	0.9300
C4—C1′	1.493 (3)	C12′—C13′	1.393 (4)
C5—C6	1.415 (3)	C12′—H12′	0.9300
C5—H5	0.9300	C13′—H13′	0.9300
C6—H6	0.9300	C14′—C16′	1.510 (3)
C1′—O1′	1.415 (2)	C14′—C15′	1.520 (3)

C1′—H1′1	0.9700	C14′—C17′	1.520 (4)
C1′—H1′2	0.9700	C15′—H15A	0.9600
C2′—C7′	1.374 (3)	C15′—H15B	0.9600
C2′—C3′	1.385 (3)	C15′—H15C	0.9600
C3′—C4′	1.381 (4)	C16′—H16A	0.9600
C3′—H3′	0.9300	C16′—H16B	0.9600
C4′—C5′	1.344 (5)	C16′—H16C	0.9600
C4′—H4′	0.9300	C17′—H17A	0.9600
C5′—C6′	1.346 (5)	C17′—H17B	0.9600
C5′—H5′	0.9300	C17′—H17C	0.9600

O1′—Si—C2′	109.06 (9)	C2′—C7′—H7′	119.2
O1′—Si—C8′	108.41 (10)	C6′—C7′—H7′	119.2
C2′—Si—C8′	110.90 (10)	C13′—C8′—C9′	116.3 (2)
O1′—Si—C14′	103.51 (9)	C13′—C8′—Si	122.96 (17)
C2′—Si—C14′	114.95 (10)	C9′—C8′—Si	120.66 (18)
C8′—Si—C14′	109.59 (10)	C10′—C9′—C8′	121.6 (3)
C6—N1—N2	115.14 (18)	C10′—C9′—H9′	119.2
N1—N2—C3	127.44 (18)	C8′—C9′—H9′	119.2
N1—N2—H2	116.9 (16)	C11′—C10′—C9′	120.1 (3)
C3—N2—H2	115.5 (16)	C11′—C10′—H10′	120.0
O3—C3—N2	120.83 (18)	C9′—C10′—H10′	120.0
O3—C3—C4	124.04 (18)	C10′—C11′—C12′	120.4 (3)
N2—C3—C4	115.12 (18)	C10′—C11′—H11′	119.8
C5—C4—C3	118.56 (18)	C12′—C11′—H11′	119.8
C5—C4—C1′	124.70 (18)	C11′—C12′—C13′	119.7 (3)
C3—C4—C1′	116.74 (17)	C11′—C12′—H12′	120.1
C4—C5—C6	119.70 (19)	C13′—C12′—H12′	120.1
C4—C5—H5	120.1	C8′—C13′—C12′	121.8 (3)
C6—C5—H5	120.1	C8′—C13′—H13′	119.1
N1—C6—C5	124.0 (2)	C12′—C13′—H13′	119.1
N1—C6—H6	118.0	C16′—C14′—C15′	108.6 (2)
C5—C6—H6	118.0	C16′—C14′—C17′	109.2 (3)
O1′—C1′—C4	109.16 (16)	C15′—C14′—C17′	108.4 (3)
O1′—C1′—H1′1	109.8	C16′—C14′—Si	110.01 (18)
C4—C1′—H1′1	109.8	C15′—C14′—Si	108.18 (16)
O1′—C1′—H1′2	109.8	C17′—C14′—Si	112.41 (17)
C4—C1′—H1′2	109.8	C14′—C15′—H15A	109.5
H1′1—C1′—H1′2	108.3	C14′—C15′—H15B	109.5
C1′—O1′—Si	125.32 (13)	H15A—C15′—H15B	109.5
C7′—C2′—C3′	115.6 (2)	C14′—C15′—H15C	109.5
C7′—C2′—Si	123.85 (18)	H15A—C15′—H15C	109.5
C3′—C2′—Si	120.58 (18)	H15B—C15′—H15C	109.5
C4′—C3′—C2′	122.3 (3)	C14′—C16′—H16A	109.5
C4′—C3′—H3′	118.8	C14′—C16′—H16B	109.5
C2′—C3′—H3′	118.8	H16A—C16′—H16B	109.5
C5′—C4′—C3′	120.3 (3)	C14′—C16′—H16C	109.5
C5′—C4′—H4′	119.8	H16A—C16′—H16C	109.5

C3′—C4′—H4′	119.8	H16B—C16′—H16C	109.5
C4′—C5′—C6′	119.3 (3)	C14′—C17′—H17A	109.5
C4′—C5′—H5′	120.3	C14′—C17′—H17B	109.5
C6′—C5′—H5′	120.3	H17A—C17′—H17B	109.5
C5′—C6′—C7′	120.8 (3)	C14′—C17′—H17C	109.5
C5′—C6′—H6′	119.6	H17A—C17′—H17C	109.5
C7′—C6′—H6′	119.6	H17B—C17′—H17C	109.5
C2′—C7′—C6′	121.6 (3)		

C6—N1—N2—C3	−0.3 (3)	C4′—C5′—C6′—C7′	1.3 (5)
N1—N2—C3—O3	−179.2 (2)	C3′—C2′—C7′—C6′	−2.0 (4)
N1—N2—C3—C4	0.9 (3)	Si—C2′—C7′—C6′	178.6 (2)
O3—C3—C4—C5	179.5 (2)	C5′—C6′—C7′—C2′	0.5 (5)
N2—C3—C4—C5	−0.7 (3)	O1′—Si—C8′—C13′	−170.38 (18)
O3—C3—C4—C1′	−0.8 (3)	C2′—Si—C8′—C13′	−50.7 (2)
N2—C3—C4—C1′	179.02 (19)	C14′—Si—C8′—C13′	77.3 (2)
C3—C4—C5—C6	0.0 (3)	O1′—Si—C8′—C9′	12.29 (19)
C1′—C4—C5—C6	−179.7 (2)	C2′—Si—C8′—C9′	132.00 (17)
N2—N1—C6—C5	−0.5 (4)	C14′—Si—C8′—C9′	−100.04 (18)
C4—C5—C6—N1	0.7 (4)	C13′—C8′—C9′—C10′	−0.1 (3)
C5—C4—C1′—O1′	−6.1 (3)	Si—C8′—C9′—C10′	177.36 (17)
C3—C4—C1′—O1′	174.22 (19)	C8′—C9′—C10′—C11′	0.8 (4)
C4—C1′—O1′—Si	−174.30 (15)	C9′—C10′—C11′—C12′	−0.8 (4)
C2′—Si—O1′—C1′	−45.6 (2)	C10′—C11′—C12′—C13′	0.2 (5)
C8′—Si—O1′—C1′	75.2 (2)	C9′—C8′—C13′—C12′	−0.5 (3)
C14′—Si—O1′—C1′	−168.44 (19)	Si—C8′—C13′—C12′	−178.0 (2)
O1′—Si—C2′—C7′	118.5 (2)	C11′—C12′—C13′—C8′	0.5 (4)
C8′—Si—C2′—C7′	−0.8 (2)	O1′—Si—C14′—C16′	−177.2 (2)
C14′—Si—C2′—C7′	−125.8 (2)	C2′—Si—C14′—C16′	64.0 (2)
O1′—Si—C2′—C3′	−60.8 (2)	C8′—Si—C14′—C16′	−61.7 (2)
C8′—Si—C2′—C3′	179.9 (2)	O1′—Si—C14′—C15′	−58.7 (2)
C14′—Si—C2′—C3′	54.9 (2)	C2′—Si—C14′—C15′	−177.52 (18)
C7′—C2′—C3′—C4′	1.8 (4)	C8′—Si—C14′—C15′	56.8 (2)
Si—C2′—C3′—C4′	−178.8 (2)	O1′—Si—C14′—C17′	61.0 (3)
C2′—C3′—C4′—C5′	−0.1 (5)	C2′—Si—C14′—C17′	−57.9 (3)
C3′—C4′—C5′—C6′	−1.5 (5)	C8′—Si—C14′—C17′	176.5 (3)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C8′–C13′ ring

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O3^{i}	0.93 (3)	1.84 (3)	2.764 (2)	176 (2)
C6—H6···*Cg*2^{ii}	0.93	2.76	3.637 (3)	138

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