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ISSN 2414-3146

# Apilimod

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Received 21 April 2017
Accepted 9 May 2017

Edited by M. Zeller, Purdue University, USA

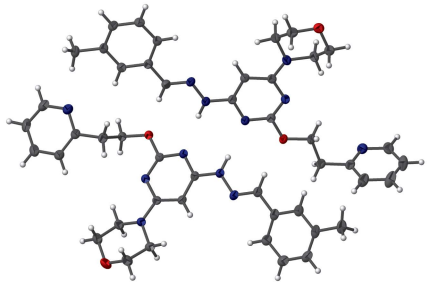
**Keywords:** crystal structure; hydrogen bonding; structural confirmation; NMR; antiviral.

**CCDC reference**: 1526003

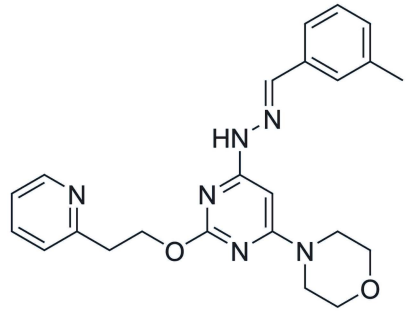
**Structural data**: full structural data are available from iucrdata.iucr.org

Apilimod {systematic name: *N*-[(*E*)-(3-methylbenzylidene)amino]-6-(morpholin-4-yl)-2-[2-(pyridin-2-yl)ethoxy]pyrimidin-4-amine}, $C_{23}H_{26}N_6O_2$, a molecule of interest for its antiviral properties, was acquired from several different commercial vendors. Analysis of several commercial batches had led to some ambiguity over the exact structure. In order to remove any ambiguity, the structure was confirmed by X-ray crystallography. In addition, the NMR spectra are provided as reference material for future investigations.

**3D view**



**Chemical scheme**




## Structure description

Apilimod is an inhibitor of IL12/23 production, originally developed for the treatment of rheumatoid arthritis by Synta pharmaceuticals (Ono *et al.*, 2003). More recently, it was disclosed that apilimod acts as an inhibitor of PIKFyve, a key enzyme which phosphorylates phosphatidylinositol 3-phosphate to phosphatidylinositol 3,5-diphosphate (Cai *et al.*, 2013). Currently, apilimod is under investigation for its antiviral activity, and recent work has shown that it has pronounced activity against the ebola virus (Cunningham, 2016; Lichenstein *et al.* 2016). However, significantly different antiviral activity was noted between different commercial batches of apilimod, which led us to a more thorough chemical characterization of the pharmaceutical. Upon further examination, it was found that there were several commercial batches where the ethoxypyridyl substituent and the morpholine substituent on the core pyrimidine ring were switched, which led to sharply diminished antiviral activity. In order to confirm the correct structure, and ensure the most active batch of apilimod was actually apilimod, single-crystal X-ray crystallography on the most biologically active commercial batch of apilimod was utilized in order to obtain an unambiguous structure.

Structural analysis shows the presence of two crystallographically independent molecules, whose connectivity matches that of the published structure (Fig. 1). Notably, the

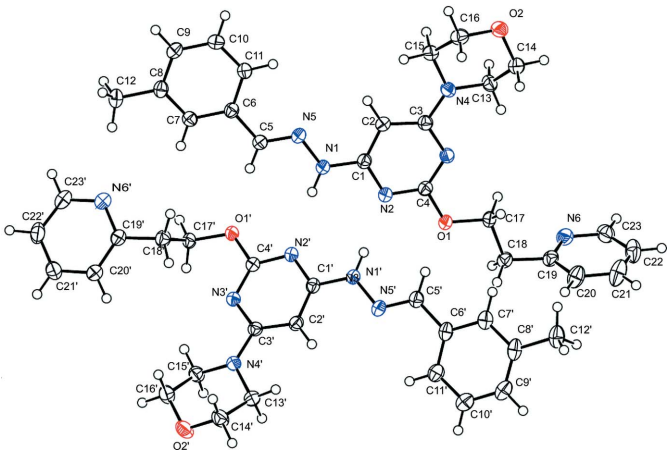



**Figure 1**
The molecular structure of the title compound, showing 50% probability displacement ellipsoids

presence of intermolecular hydrogen bonding between the NH of the hydrazine functionality and the pyrimidine nitrogen atom is present, with a hydrogen-bond length of 3.0626 (16) Å apparent (Table 1). The structures of the two molecules differ slightly in several ways, with the most distinct point of deviation being the O1—C17—C18 angle, which measures 106.76 (10)°, while the corresponding O1′—C17′—C18′ angle is 111.53 (11)°. As expected, in both structures the imine bond maintains an (*E*) geometry.

## Synthesis and crystallization

Apilimod was provided by Axon Medchem (Reston, VA) and synthesized *via* the route outlined in the original patent (Ono *et al.*, 2003). The compound was crystallized as colorless blocks by dissolving a sample of approximately 1 mg in 0.35 ml dichloromethane and vapor diffusing the sample with pentane over two days. In addition to X-ray crystallography, the

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···N2′ | 0.91 (1) | 2.16 (1) | 3.0626 (16) | 169 (1) |
| N1′—H1′···N2 | 0.92 (1) | 2.10 (1) | 3.0129 (16) | 178 (2) |

compound was characterized by $^{1}$H NMR and $^{13}$C NMR. For reference, those values and spectra are reproduced here (Figs. 2 and 3). Notably, apilimod shows the morpholine peaks as two distinct peaks at 3.78 and 3.64 p.p.m. This is a key difference, as the incorrect regioisomeric structure shows a single morpholine peak.

$^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.65 (*s*, 1H), 8.54 (*ddd*, *J* = 4.9, 1.9, 0.9 Hz, 1H), 7.74 (*s*, 1H), 7.60 (*td*, *J* = 7.7, 1.9 Hz, 1H), 7.54–7.39 (*m*, 2H), 7.32–7.23 (*m*, 1H), 7.20–7.08 (*m*, 2H), 6.08 (*s*, 1H), 4.65 (*t*, *J* = 6.9 Hz, 2H), 3.78 (*dd*, *J* = 5.7, 4.0 Hz, 4H), 3.64 (*dd*, *J* = 5.7, 4.1 Hz, 4H), 3.26 (*t*, *J* = 6.9 Hz, 2H), 2.38 (*s*, 3H).

$^{13}$C NMR (101 MHz, $CDCl_3$) $\delta$ 164.7, 163.9, 162.7, 158.7, 149.4, 142.0, 138.5, 136.7, 134.3, 130.5, 128.7, 127.4, 124.2, 124.0, 121.7, 76.5, 66.8, 66.2, 44.8, 37.9, 21.5.

## Refinement

Crystal data, data collection and structural refinement details are summarized in Table 2.

## Acknowledgements

The authors would like to thank Judith M. White, Julie Dyall, Elizabeth A. Nelson, Gene G. Olinger Jr and Lisa Dewald at the University of Virginia and at the National Institute of Allergy and Infectious Diseases for leading the research that led to the discovery of the discrepancy. The authors would also like to thank the intramural research program at the National Center for Advancing Translational Studies for funding and

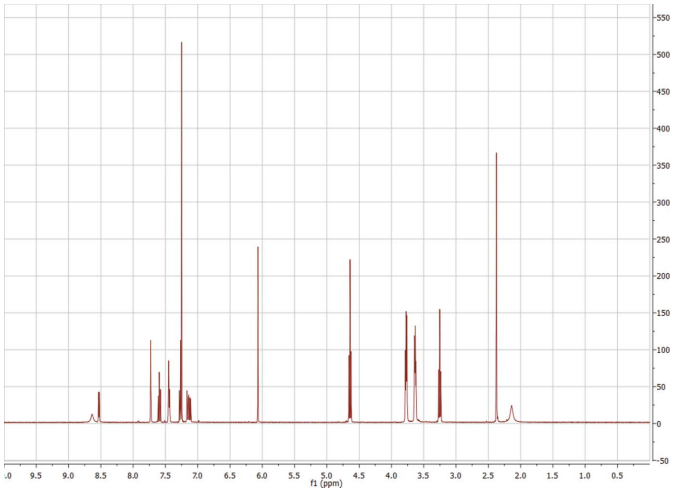


**Figure 2**
The $^{1}$H NMR spectrum of the title compound in deuterated chloroform. Note the clear splitting of the morphiline peaks at 3.78 and 3.64 p.p.m..

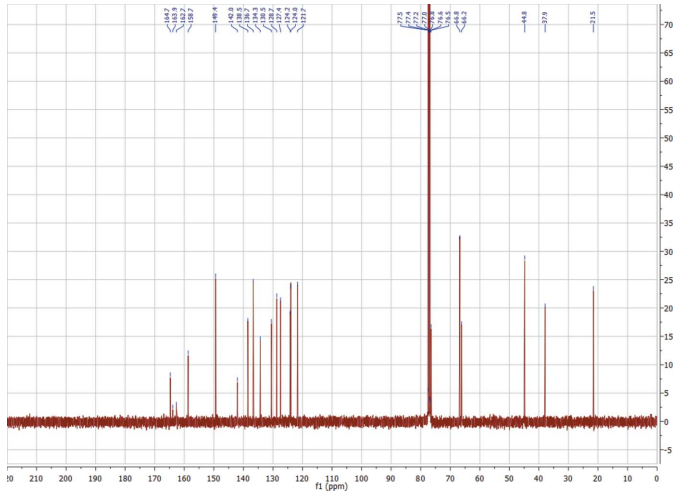


**Figure 3**
$^{13}$C NMR spectrum of the title compound in deuterated chloroform

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{23}H_{26}N_6O_2$ |
| $M_r$ | 418.50 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 100 |
| $a$, $b$, $c$ (Å) | 14.9353 (5), 15.0367 (5), 19.4231 (7) |
| $\beta$ (°) | 98.130 (2) |
| $V$ (Å$^3$) | 4318.2 (3) |
| $Z$ | 8 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.69 |
| Crystal size (mm) | 0.25 × 0.21 × 0.19 |
| | |
| Data collection | |
| Diffractometer | Bruker X8 APEXII |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2014) |
| $T_{min}$, $T_{max}$ | 0.228, 0.320 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 50098, 7881, 6816 |
| $R_{int}$ | 0.038 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.604 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.038, 0.103, 1.04 |
| No. of reflections | 7881 |
| No. of parameters | 569 |
| No. of restraints | 2 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.29, −0.22 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

the UCSD crystallography facility for the X-ray data collection.

## Funding information

Funding for this research was provided by: National Institutes of Health, National Center for Advancing Translational Sciences.

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# full crystallographic data

*IUCrData* (2017). **2**, x170693 [https://doi.org/10.1107/S2414314617006939]

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***N*-[(*E*)-(3-Methylbenzylidene)amino]-6-(morpholin-4-yl)-2-[2-(pyridin-2-yl)ethoxy]pyrimidin-4-amine**

*Crystal data*

$C_{23}H_{26}N_6O_2$
$M_r$ = 418.50
Monoclinic, $P2_1/c$
$a$ = 14.9353 (5) Å
$b$ = 15.0367 (5) Å
$c$ = 19.4231 (7) Å
$\beta$ = 98.130 (2)°
$V$ = 4318.2 (3) Å$^3$
$Z$ = 8
$F(000)$ = 1776
$D_x$ = 1.287 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54178 Å
Cell parameters from 9651 reflections
$\theta$ = 4.2–68.5°
$\mu$ = 0.69 mm$^{-1}$
$T$ = 100 K
Block, colourless
0.25 × 0.21 × 0.19 mm

*Data collection*

Bruker X8 APEXII diffractometer
Radiation source: Micro Focus Rotating Anode, Bruker Microstar FR-592
Double Bounce Multilayer Mirrors monochromator
Detector resolution: 7.9 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
$T_{min}$ = 0.228, $T_{max}$ = 0.320
50098 measured reflections
7881 independent reflections
6816 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.038
$\theta_{max}$ = 68.5°, $\theta_{min}$ = 3.0°
$h$ = −17→18
$k$ = −18→17
$l$ = −23→22

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
$S$ = 1.04
7881 reflections
569 parameters
2 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2 + 1.2958P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. All nonhydrogen atoms were refined anisotropically by full-matrix least-squares (*SHELXL2014*). All carbon bonded hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in *SHELXL2014*. All other hydrogen atoms (H-bonding) were located in difference mapa. Their relative positions were restrained using *DFIX* commands and their thermal parameters freely refined.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.34895 (6) | 0.49264 (6) | 0.73640 (4) | 0.0263 (2) |
| O2 | 0.79885 (6) | 0.64234 (7) | 0.75289 (5) | 0.0313 (2) |
| N1 | 0.35964 (8) | 0.58848 (8) | 0.51765 (6) | 0.0277 (2) |
| H1 | 0.2990 (9) | 0.5779 (11) | 0.5100 (8) | 0.031 (4)* |
| N2 | 0.35530 (7) | 0.54354 (7) | 0.62910 (5) | 0.0247 (2) |
| N3 | 0.48892 (7) | 0.53447 (7) | 0.71298 (5) | 0.0240 (2) |
| N4 | 0.62723 (8) | 0.58340 (8) | 0.68986 (6) | 0.0301 (3) |
| N5 | 0.40438 (7) | 0.62175 (7) | 0.46652 (5) | 0.0255 (2) |
| N6 | 0.41499 (8) | 0.34602 (8) | 0.92805 (6) | 0.0325 (3) |
| C1 | 0.40704 (9) | 0.57268 (9) | 0.58201 (6) | 0.0242 (3) |
| C2 | 0.49980 (9) | 0.58574 (9) | 0.59747 (7) | 0.0263 (3) |
| H2 | 0.5349 | 0.6060 | 0.5634 | 0.032* |
| C3 | 0.53853 (9) | 0.56760 (9) | 0.66551 (7) | 0.0245 (3) |
| C4 | 0.40211 (9) | 0.52482 (8) | 0.69093 (6) | 0.0232 (3) |
| C5 | 0.35753 (9) | 0.63339 (9) | 0.40663 (7) | 0.0256 (3) |
| H5 | 0.2947 | 0.6200 | 0.4001 | 0.031* |
| C6 | 0.39974 (9) | 0.66702 (9) | 0.34817 (6) | 0.0241 (3) |
| C7 | 0.34625 (9) | 0.67965 (9) | 0.28399 (7) | 0.0250 (3) |
| H7 | 0.2829 | 0.6698 | 0.2802 | 0.030* |
| C8 | 0.38319 (9) | 0.70632 (9) | 0.22533 (7) | 0.0262 (3) |
| C9 | 0.47498 (9) | 0.72490 (9) | 0.23255 (7) | 0.0286 (3) |
| H9 | 0.5014 | 0.7447 | 0.1935 | 0.034* |
| C10 | 0.52836 (9) | 0.71475 (10) | 0.29639 (7) | 0.0297 (3) |
| H10 | 0.5909 | 0.7290 | 0.3008 | 0.036* |
| C11 | 0.49266 (9) | 0.68427 (9) | 0.35387 (7) | 0.0262 (3) |
| H11 | 0.5307 | 0.6751 | 0.3968 | 0.031* |
| C12 | 0.32505 (10) | 0.71098 (10) | 0.15531 (7) | 0.0342 (3) |
| H12A | 0.3463 | 0.6672 | 0.1239 | 0.051* |
| H12B | 0.3289 | 0.7707 | 0.1358 | 0.051* |
| H12C | 0.2621 | 0.6981 | 0.1607 | 0.051* |
| C13 | 0.68901 (9) | 0.62522 (10) | 0.64810 (7) | 0.0313 (3) |
| H13A | 0.6545 | 0.6593 | 0.6096 | 0.038* |
| H13B | 0.7249 | 0.5792 | 0.6278 | 0.038* |
| C14 | 0.75126 (10) | 0.68681 (10) | 0.69423 (7) | 0.0327 (3) |
| H14A | 0.7954 | 0.7134 | 0.6667 | 0.039* |
| H14B | 0.7152 | 0.7358 | 0.7105 | 0.039* |
| C15 | 0.67356 (9) | 0.53962 (9) | 0.75186 (7) | 0.0286 (3) |
| H15A | 0.7084 | 0.4882 | 0.7381 | 0.034* |
| H15B | 0.6285 | 0.5172 | 0.7804 | 0.034* |
| C16 | 0.73665 (9) | 0.60377 (10) | 0.79406 (7) | 0.0301 (3) |

| | | | | |
|---|---|---|---|---|
| H16A | 0.7009 | 0.6515 | 0.8124 | 0.036* |
| H16B | 0.7707 | 0.5721 | 0.8342 | 0.036* |
| C17 | 0.39265 (9) | 0.47784 (9) | 0.80631 (6) | 0.0267 (3) |
| H17A | 0.4170 | 0.5344 | 0.8274 | 0.032* |
| H17B | 0.4432 | 0.4352 | 0.8065 | 0.032* |
| C18 | 0.32146 (9) | 0.44048 (9) | 0.84671 (7) | 0.0276 (3) |
| H18A | 0.2722 | 0.4844 | 0.8474 | 0.033* |
| H18B | 0.2952 | 0.3857 | 0.8238 | 0.033* |
| C19 | 0.36342 (9) | 0.41962 (9) | 0.91997 (7) | 0.0275 (3) |
| C20 | 0.35200 (12) | 0.47483 (10) | 0.97472 (8) | 0.0402 (4) |
| H20 | 0.3147 | 0.5261 | 0.9673 | 0.048* |
| C21 | 0.39550 (14) | 0.45474 (12) | 1.04074 (8) | 0.0497 (4) |
| H21 | 0.3889 | 0.4922 | 1.0791 | 0.060* |
| C22 | 0.44831 (12) | 0.37974 (11) | 1.04972 (8) | 0.0435 (4) |
| H22 | 0.4786 | 0.3641 | 1.0944 | 0.052* |
| C23 | 0.45640 (10) | 0.32763 (11) | 0.99250 (8) | 0.0378 (3) |
| H23 | 0.4932 | 0.2759 | 0.9990 | 0.045* |
| O1′ | 0.14106 (6) | 0.53264 (6) | 0.39198 (4) | 0.0257 (2) |
| O2′ | −0.28751 (7) | 0.71945 (7) | 0.41569 (5) | 0.0376 (2) |
| N1′ | 0.16456 (8) | 0.61288 (8) | 0.61828 (5) | 0.0257 (2) |
| H1′ | 0.2222 (10) | 0.5909 (12) | 0.6227 (9) | 0.039 (5)* |
| N2′ | 0.15315 (7) | 0.57612 (7) | 0.50314 (5) | 0.0231 (2) |
| N3′ | 0.01224 (7) | 0.58701 (7) | 0.42790 (5) | 0.0227 (2) |
| N4′ | −0.11443 (7) | 0.64966 (8) | 0.46210 (6) | 0.0266 (2) |
| N5′ | 0.12430 (8) | 0.63141 (7) | 0.67570 (5) | 0.0257 (2) |
| N6′ | 0.09634 (8) | 0.58164 (9) | 0.16839 (6) | 0.0349 (3) |
| C1′ | 0.11114 (9) | 0.60824 (8) | 0.55523 (6) | 0.0229 (3) |
| C2′ | 0.02131 (9) | 0.63494 (9) | 0.54633 (7) | 0.0240 (3) |
| H2′ | −0.0058 | 0.6597 | 0.5834 | 0.029* |
| C3′ | −0.02685 (9) | 0.62349 (8) | 0.48016 (6) | 0.0226 (3) |
| C4′ | 0.09872 (9) | 0.56733 (8) | 0.44311 (6) | 0.0223 (3) |
| C5′ | 0.17579 (9) | 0.63390 (9) | 0.73411 (7) | 0.0270 (3) |
| H5′ | 0.2391 | 0.6254 | 0.7358 | 0.032* |
| C6′ | 0.13749 (10) | 0.64987 (9) | 0.79854 (7) | 0.0277 (3) |
| C7′ | 0.19622 (10) | 0.66530 (9) | 0.85979 (7) | 0.0300 (3) |
| H7′ | 0.2597 | 0.6643 | 0.8590 | 0.036* |
| C8′ | 0.16319 (11) | 0.68225 (9) | 0.92267 (7) | 0.0326 (3) |
| C9′ | 0.07049 (11) | 0.68297 (10) | 0.92257 (7) | 0.0347 (3) |
| H9′ | 0.0470 | 0.6949 | 0.9646 | 0.042* |
| C10′ | 0.01152 (11) | 0.66672 (10) | 0.86247 (8) | 0.0345 (3) |
| H10′ | −0.0518 | 0.6670 | 0.8637 | 0.041* |
| C11′ | 0.04427 (10) | 0.65000 (9) | 0.80046 (7) | 0.0304 (3) |
| H11′ | 0.0034 | 0.6387 | 0.7593 | 0.037* |
| C12′ | 0.22766 (12) | 0.69882 (11) | 0.98798 (8) | 0.0401 (4) |
| H12D | 0.2258 | 0.6485 | 1.0198 | 0.060* |
| H12E | 0.2102 | 0.7534 | 1.0103 | 0.060* |
| H12F | 0.2891 | 0.7054 | 0.9765 | 0.060* |
| C13′ | −0.16680 (10) | 0.69041 (11) | 0.51118 (7) | 0.0329 (3) |

| | | | | |
|---|---|---|---|---|
| H13C | −0.1259 | 0.7202 | 0.5487 | 0.040* |
| H13D | −0.2015 | 0.6443 | 0.5324 | 0.040* |
| C14′ | −0.23092 (10) | 0.75771 (11) | 0.47298 (8) | 0.0366 (3) |
| H14C | −0.2691 | 0.7834 | 0.5057 | 0.044* |
| H14D | −0.1954 | 0.8066 | 0.4561 | 0.044* |
| C15′ | −0.17133 (9) | 0.61136 (9) | 0.40220 (7) | 0.0283 (3) |
| H15C | −0.2069 | 0.5613 | 0.4174 | 0.034* |
| H15D | −0.1330 | 0.5881 | 0.3687 | 0.034* |
| C16′ | −0.23406 (10) | 0.68121 (10) | 0.36784 (7) | 0.0337 (3) |
| H16C | −0.1983 | 0.7285 | 0.3490 | 0.040* |
| H16D | −0.2744 | 0.6544 | 0.3285 | 0.040* |
| C17′ | 0.08812 (9) | 0.52409 (9) | 0.32382 (6) | 0.0252 (3) |
| H17C | 0.0283 | 0.4984 | 0.3287 | 0.030* |
| H17D | 0.1191 | 0.4829 | 0.2952 | 0.030* |
| C18′ | 0.07489 (10) | 0.61360 (9) | 0.28716 (7) | 0.0291 (3) |
| H18C | 0.0332 | 0.6506 | 0.3103 | 0.035* |
| H18D | 0.1337 | 0.6449 | 0.2907 | 0.035* |
| C19′ | 0.03685 (9) | 0.60182 (9) | 0.21177 (7) | 0.0275 (3) |
| C20′ | −0.05490 (10) | 0.60954 (11) | 0.18879 (8) | 0.0372 (3) |
| H20′ | −0.0956 | 0.6231 | 0.2207 | 0.045* |
| C21′ | −0.08694 (11) | 0.59735 (12) | 0.11920 (8) | 0.0428 (4) |
| H21′ | −0.1497 | 0.6025 | 0.1026 | 0.051* |
| C22′ | −0.02636 (12) | 0.57763 (12) | 0.07445 (8) | 0.0411 (4) |
| H22′ | −0.0460 | 0.5694 | 0.0262 | 0.049* |
| C23′ | 0.06354 (11) | 0.57011 (12) | 0.10134 (8) | 0.0413 (4) |
| H23′ | 0.1051 | 0.5558 | 0.0702 | 0.050* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0243 (5) | 0.0343 (5) | 0.0202 (4) | −0.0029 (4) | 0.0029 (3) | 0.0037 (4) |
| O2 | 0.0267 (5) | 0.0350 (5) | 0.0321 (5) | −0.0038 (4) | 0.0037 (4) | −0.0031 (4) |
| N1 | 0.0222 (6) | 0.0399 (7) | 0.0209 (5) | −0.0032 (5) | 0.0028 (4) | 0.0033 (5) |
| N2 | 0.0239 (5) | 0.0290 (6) | 0.0211 (5) | −0.0002 (4) | 0.0032 (4) | 0.0015 (4) |
| N3 | 0.0234 (5) | 0.0251 (6) | 0.0232 (5) | −0.0010 (4) | 0.0020 (4) | 0.0013 (4) |
| N4 | 0.0224 (6) | 0.0394 (7) | 0.0279 (6) | −0.0029 (5) | 0.0013 (5) | 0.0089 (5) |
| N5 | 0.0267 (6) | 0.0297 (6) | 0.0207 (5) | −0.0007 (5) | 0.0055 (4) | 0.0010 (4) |
| N6 | 0.0327 (6) | 0.0346 (7) | 0.0309 (6) | 0.0007 (5) | 0.0071 (5) | 0.0060 (5) |
| C1 | 0.0262 (7) | 0.0251 (6) | 0.0214 (6) | 0.0011 (5) | 0.0035 (5) | −0.0006 (5) |
| C2 | 0.0247 (7) | 0.0311 (7) | 0.0237 (6) | −0.0001 (5) | 0.0056 (5) | 0.0024 (5) |
| C3 | 0.0245 (6) | 0.0238 (6) | 0.0252 (6) | 0.0007 (5) | 0.0034 (5) | 0.0008 (5) |
| C4 | 0.0249 (6) | 0.0231 (6) | 0.0220 (6) | −0.0014 (5) | 0.0044 (5) | −0.0008 (5) |
| C5 | 0.0240 (6) | 0.0293 (7) | 0.0236 (6) | −0.0013 (5) | 0.0038 (5) | −0.0009 (5) |
| C6 | 0.0264 (7) | 0.0239 (6) | 0.0221 (6) | −0.0008 (5) | 0.0038 (5) | −0.0019 (5) |
| C7 | 0.0239 (6) | 0.0249 (7) | 0.0259 (6) | −0.0006 (5) | 0.0024 (5) | 0.0001 (5) |
| C8 | 0.0321 (7) | 0.0226 (6) | 0.0234 (6) | 0.0023 (5) | 0.0023 (5) | 0.0006 (5) |
| C9 | 0.0331 (7) | 0.0285 (7) | 0.0256 (7) | −0.0010 (6) | 0.0086 (5) | 0.0030 (5) |
| C10 | 0.0242 (7) | 0.0339 (7) | 0.0314 (7) | −0.0026 (5) | 0.0055 (5) | 0.0004 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C11 | 0.0258 (7) | 0.0289 (7) | 0.0235 (6) | −0.0007 (5) | 0.0018 (5) | −0.0013 (5) |
| C12 | 0.0379 (8) | 0.0400 (8) | 0.0235 (7) | 0.0014 (6) | 0.0000 (6) | 0.0045 (6) |
| C13 | 0.0246 (7) | 0.0401 (8) | 0.0294 (7) | −0.0021 (6) | 0.0046 (5) | 0.0053 (6) |
| C14 | 0.0313 (7) | 0.0322 (8) | 0.0356 (8) | −0.0016 (6) | 0.0086 (6) | 0.0018 (6) |
| C15 | 0.0262 (7) | 0.0297 (7) | 0.0286 (7) | 0.0003 (5) | −0.0006 (5) | 0.0041 (5) |
| C16 | 0.0299 (7) | 0.0314 (7) | 0.0290 (7) | −0.0005 (6) | 0.0038 (6) | −0.0009 (6) |
| C17 | 0.0278 (7) | 0.0321 (7) | 0.0198 (6) | −0.0021 (5) | 0.0015 (5) | 0.0031 (5) |
| C18 | 0.0292 (7) | 0.0288 (7) | 0.0252 (7) | −0.0014 (5) | 0.0053 (5) | 0.0028 (5) |
| C19 | 0.0301 (7) | 0.0270 (7) | 0.0261 (7) | −0.0042 (5) | 0.0068 (5) | 0.0046 (5) |
| C20 | 0.0618 (10) | 0.0292 (8) | 0.0303 (8) | 0.0036 (7) | 0.0090 (7) | 0.0023 (6) |
| C21 | 0.0840 (13) | 0.0380 (9) | 0.0266 (8) | −0.0095 (9) | 0.0064 (8) | −0.0022 (7) |
| C22 | 0.0544 (10) | 0.0415 (9) | 0.0308 (8) | −0.0155 (8) | −0.0066 (7) | 0.0106 (7) |
| C23 | 0.0334 (8) | 0.0400 (8) | 0.0392 (8) | −0.0015 (6) | 0.0019 (6) | 0.0129 (7) |
| O1′ | 0.0230 (4) | 0.0346 (5) | 0.0192 (4) | 0.0046 (4) | 0.0018 (3) | −0.0038 (4) |
| O2′ | 0.0268 (5) | 0.0451 (6) | 0.0387 (6) | 0.0091 (4) | −0.0036 (4) | −0.0094 (5) |
| N1′ | 0.0241 (6) | 0.0339 (6) | 0.0190 (5) | 0.0018 (5) | 0.0030 (4) | −0.0023 (4) |
| N2′ | 0.0233 (5) | 0.0268 (6) | 0.0192 (5) | 0.0002 (4) | 0.0025 (4) | −0.0007 (4) |
| N3′ | 0.0223 (5) | 0.0244 (5) | 0.0212 (5) | 0.0009 (4) | 0.0028 (4) | −0.0004 (4) |
| N4′ | 0.0226 (6) | 0.0355 (6) | 0.0217 (5) | 0.0044 (5) | 0.0026 (4) | −0.0027 (5) |
| N5′ | 0.0302 (6) | 0.0274 (6) | 0.0199 (5) | 0.0002 (5) | 0.0050 (4) | −0.0014 (4) |
| N6′ | 0.0321 (6) | 0.0459 (7) | 0.0277 (6) | 0.0008 (5) | 0.0071 (5) | 0.0016 (5) |
| C1′ | 0.0257 (6) | 0.0224 (6) | 0.0204 (6) | −0.0021 (5) | 0.0027 (5) | 0.0010 (5) |
| C2′ | 0.0258 (6) | 0.0254 (6) | 0.0214 (6) | 0.0015 (5) | 0.0052 (5) | −0.0001 (5) |
| C3′ | 0.0225 (6) | 0.0221 (6) | 0.0234 (6) | 0.0001 (5) | 0.0045 (5) | 0.0023 (5) |
| C4′ | 0.0233 (6) | 0.0228 (6) | 0.0209 (6) | −0.0002 (5) | 0.0039 (5) | 0.0002 (5) |
| C5′ | 0.0303 (7) | 0.0274 (7) | 0.0232 (6) | 0.0012 (5) | 0.0028 (5) | −0.0008 (5) |
| C6′ | 0.0388 (8) | 0.0223 (6) | 0.0213 (6) | 0.0010 (5) | 0.0021 (5) | −0.0005 (5) |
| C7′ | 0.0378 (8) | 0.0260 (7) | 0.0255 (7) | 0.0011 (6) | 0.0017 (6) | 0.0001 (5) |
| C8′ | 0.0527 (9) | 0.0219 (7) | 0.0218 (7) | 0.0025 (6) | −0.0002 (6) | −0.0001 (5) |
| C9′ | 0.0498 (9) | 0.0288 (7) | 0.0276 (7) | 0.0044 (6) | 0.0126 (6) | 0.0011 (6) |
| C10′ | 0.0399 (8) | 0.0319 (8) | 0.0333 (8) | 0.0011 (6) | 0.0108 (6) | 0.0001 (6) |
| C11′ | 0.0366 (8) | 0.0275 (7) | 0.0276 (7) | −0.0010 (6) | 0.0060 (6) | −0.0010 (5) |
| C12′ | 0.0543 (10) | 0.0376 (8) | 0.0264 (7) | 0.0030 (7) | −0.0016 (7) | −0.0041 (6) |
| C13′ | 0.0284 (7) | 0.0446 (8) | 0.0266 (7) | 0.0059 (6) | 0.0066 (6) | −0.0031 (6) |
| C14′ | 0.0304 (7) | 0.0437 (9) | 0.0340 (8) | 0.0086 (6) | −0.0008 (6) | −0.0090 (6) |
| C15′ | 0.0251 (7) | 0.0308 (7) | 0.0280 (7) | 0.0002 (5) | 0.0006 (5) | −0.0021 (5) |
| C16′ | 0.0336 (8) | 0.0361 (8) | 0.0295 (7) | 0.0056 (6) | −0.0024 (6) | −0.0037 (6) |
| C17′ | 0.0254 (6) | 0.0305 (7) | 0.0191 (6) | 0.0015 (5) | 0.0012 (5) | −0.0044 (5) |
| C18′ | 0.0315 (7) | 0.0309 (7) | 0.0248 (7) | −0.0020 (6) | 0.0034 (5) | −0.0014 (5) |
| C19′ | 0.0302 (7) | 0.0277 (7) | 0.0250 (7) | −0.0009 (5) | 0.0055 (5) | 0.0022 (5) |
| C20′ | 0.0297 (7) | 0.0537 (10) | 0.0290 (7) | 0.0014 (7) | 0.0069 (6) | 0.0074 (7) |
| C21′ | 0.0316 (8) | 0.0612 (11) | 0.0335 (8) | −0.0050 (7) | −0.0020 (6) | 0.0124 (7) |
| C22′ | 0.0485 (9) | 0.0504 (10) | 0.0227 (7) | −0.0061 (7) | −0.0009 (6) | 0.0052 (6) |
| C23′ | 0.0451 (9) | 0.0549 (10) | 0.0257 (7) | 0.0013 (7) | 0.0115 (6) | −0.0005 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C4 | 1.3575 (15) | O1′—C4′ | 1.3549 (15) |
| O1—C17 | 1.4381 (15) | O1′—C17′ | 1.4486 (15) |
| O2—C14 | 1.4217 (17) | O2′—C14′ | 1.4204 (17) |
| O2—C16 | 1.4313 (17) | O2′—C16′ | 1.4289 (17) |
| N1—H1 | 0.911 (13) | N1′—H1′ | 0.915 (14) |
| N1—N5 | 1.3678 (15) | N1′—N5′ | 1.3684 (15) |
| N1—C1 | 1.3673 (17) | N1′—C1′ | 1.3656 (16) |
| N2—C1 | 1.3513 (17) | N2′—C1′ | 1.3527 (16) |
| N2—C4 | 1.3314 (17) | N2′—C4′ | 1.3303 (16) |
| N3—C3 | 1.3566 (17) | N3′—C3′ | 1.3564 (16) |
| N3—C4 | 1.3147 (17) | N3′—C4′ | 1.3172 (17) |
| N4—C3 | 1.3631 (18) | N4′—C3′ | 1.3635 (17) |
| N4—C13 | 1.4548 (17) | N4′—C13′ | 1.4515 (17) |
| N4—C15 | 1.4583 (17) | N4′—C15′ | 1.4587 (17) |
| N5—C5 | 1.2819 (17) | N5′—C5′ | 1.2781 (17) |
| N6—C19 | 1.3448 (19) | N6′—C19′ | 1.3429 (18) |
| N6—C23 | 1.3443 (19) | N6′—C23′ | 1.3363 (19) |
| C1—C2 | 1.3893 (19) | C1′—C2′ | 1.3877 (18) |
| C2—H2 | 0.9500 | C2′—H2′ | 0.9500 |
| C2—C3 | 1.3925 (18) | C2′—C3′ | 1.3918 (18) |
| C5—H5 | 0.9500 | C5′—H5′ | 0.9500 |
| C5—C6 | 1.4645 (18) | C5′—C6′ | 1.4675 (18) |
| C6—C7 | 1.3952 (18) | C6′—C7′ | 1.3940 (19) |
| C6—C11 | 1.4008 (19) | C6′—C11′ | 1.398 (2) |
| C7—H7 | 0.9500 | C7′—H7′ | 0.9500 |
| C7—C8 | 1.3932 (18) | C7′—C8′ | 1.404 (2) |
| C8—C9 | 1.387 (2) | C8′—C9′ | 1.384 (2) |
| C8—C12 | 1.5083 (18) | C8′—C12′ | 1.501 (2) |
| C9—H9 | 0.9500 | C9′—H9′ | 0.9500 |
| C9—C10 | 1.3843 (19) | C9′—C10′ | 1.381 (2) |
| C10—H10 | 0.9500 | C10′—H10′ | 0.9500 |
| C10—C11 | 1.3818 (19) | C10′—C11′ | 1.386 (2) |
| C11—H11 | 0.9500 | C11′—H11′ | 0.9500 |
| C12—H12A | 0.9800 | C12′—H12D | 0.9800 |
| C12—H12B | 0.9800 | C12′—H12E | 0.9800 |
| C12—H12C | 0.9800 | C12′—H12F | 0.9800 |
| C13—H13A | 0.9900 | C13′—H13C | 0.9900 |
| C13—H13B | 0.9900 | C13′—H13D | 0.9900 |
| C13—C14 | 1.513 (2) | C13′—C14′ | 1.513 (2) |
| C14—H14A | 0.9900 | C14′—H14C | 0.9900 |
| C14—H14B | 0.9900 | C14′—H14D | 0.9900 |
| C15—H15A | 0.9900 | C15′—H15C | 0.9900 |
| C15—H15B | 0.9900 | C15′—H15D | 0.9900 |
| C15—C16 | 1.5071 (19) | C15′—C16′ | 1.500 (2) |
| C16—H16A | 0.9900 | C16′—H16C | 0.9900 |
| C16—H16B | 0.9900 | C16′—H16D | 0.9900 |

| | | | |
|---|---|---|---|
| C17—H17A | 0.9900 | C17′—H17C | 0.9900 |
| C17—H17B | 0.9900 | C17′—H17D | 0.9900 |
| C17—C18 | 1.5159 (18) | C17′—C18′ | 1.5225 (19) |
| C18—H18A | 0.9900 | C18′—H18C | 0.9900 |
| C18—H18B | 0.9900 | C18′—H18D | 0.9900 |
| C18—C19 | 1.5045 (18) | C18′—C19′ | 1.5044 (18) |
| C19—C20 | 1.379 (2) | C19′—C20′ | 1.385 (2) |
| C20—H20 | 0.9500 | C20′—H20′ | 0.9500 |
| C20—C21 | 1.386 (2) | C20′—C21′ | 1.381 (2) |
| C21—H21 | 0.9500 | C21′—H21′ | 0.9500 |
| C21—C22 | 1.373 (3) | C21′—C22′ | 1.373 (2) |
| C22—H22 | 0.9500 | C22′—H22′ | 0.9500 |
| C22—C23 | 1.379 (2) | C22′—C23′ | 1.375 (2) |
| C23—H23 | 0.9500 | C23′—H23′ | 0.9500 |
| | | | |
| C4—O1—C17 | 116.13 (10) | C4′—O1′—C17′ | 116.94 (10) |
| C14—O2—C16 | 110.36 (10) | C14′—O2′—C16′ | 110.32 (11) |
| N5—N1—H1 | 121.4 (10) | N5′—N1′—H1′ | 120.9 (11) |
| C1—N1—H1 | 119.6 (10) | C1′—N1′—H1′ | 119.2 (11) |
| C1—N1—N5 | 118.97 (11) | C1′—N1′—N5′ | 118.22 (11) |
| C4—N2—C1 | 113.68 (11) | C4′—N2′—C1′ | 113.60 (11) |
| C4—N3—C3 | 115.31 (11) | C4′—N3′—C3′ | 115.79 (11) |
| C3—N4—C13 | 122.94 (11) | C3′—N4′—C13′ | 122.64 (11) |
| C3—N4—C15 | 122.16 (11) | C3′—N4′—C15′ | 121.38 (11) |
| C13—N4—C15 | 113.03 (11) | C13′—N4′—C15′ | 112.53 (11) |
| C5—N5—N1 | 116.67 (11) | C5′—N5′—N1′ | 116.79 (11) |
| C23—N6—C19 | 117.29 (13) | C23′—N6′—C19′ | 117.19 (13) |
| N1—C1—C2 | 123.00 (12) | N1′—C1′—C2′ | 121.93 (11) |
| N2—C1—N1 | 113.80 (11) | N2′—C1′—N1′ | 114.52 (11) |
| N2—C1—C2 | 123.20 (12) | N2′—C1′—C2′ | 123.54 (11) |
| C1—C2—H2 | 121.8 | C1′—C2′—H2′ | 121.8 |
| C1—C2—C3 | 116.44 (12) | C1′—C2′—C3′ | 116.33 (11) |
| C3—C2—H2 | 121.8 | C3′—C2′—H2′ | 121.8 |
| N3—C3—N4 | 115.19 (11) | N3′—C3′—N4′ | 115.02 (11) |
| N3—C3—C2 | 121.56 (12) | N3′—C3′—C2′ | 121.34 (11) |
| N4—C3—C2 | 123.24 (12) | N4′—C3′—C2′ | 123.61 (12) |
| N2—C4—O1 | 112.42 (11) | N2′—C4′—O1′ | 112.95 (11) |
| N3—C4—O1 | 117.91 (11) | N3′—C4′—O1′ | 117.81 (11) |
| N3—C4—N2 | 129.66 (12) | N3′—C4′—N2′ | 129.24 (11) |
| N5—C5—H5 | 119.6 | N5′—C5′—H5′ | 119.9 |
| N5—C5—C6 | 120.74 (12) | N5′—C5′—C6′ | 120.24 (13) |
| C6—C5—H5 | 119.6 | C6′—C5′—H5′ | 119.9 |
| C7—C6—C5 | 119.00 (12) | C7′—C6′—C5′ | 118.75 (13) |
| C7—C6—C11 | 118.76 (12) | C7′—C6′—C11′ | 119.07 (12) |
| C11—C6—C5 | 122.21 (12) | C11′—C6′—C5′ | 122.18 (12) |
| C6—C7—H7 | 119.1 | C6′—C7′—H7′ | 119.4 |
| C8—C7—C6 | 121.80 (12) | C6′—C7′—C8′ | 121.10 (14) |
| C8—C7—H7 | 119.1 | C8′—C7′—H7′ | 119.4 |

| | | | |
|---|---|---|---|
| C7—C8—C12 | 120.45 (12) | C7′—C8′—C12′ | 120.20 (14) |
| C9—C8—C7 | 118.39 (12) | C9′—C8′—C7′ | 118.34 (13) |
| C9—C8—C12 | 121.11 (12) | C9′—C8′—C12′ | 121.46 (13) |
| C8—C9—H9 | 119.9 | C8′—C9′—H9′ | 119.4 |
| C10—C9—C8 | 120.28 (12) | C10′—C9′—C8′ | 121.20 (13) |
| C10—C9—H9 | 119.9 | C10′—C9′—H9′ | 119.4 |
| C9—C10—H10 | 119.3 | C9′—C10′—H10′ | 119.8 |
| C11—C10—C9 | 121.41 (12) | C9′—C10′—C11′ | 120.37 (14) |
| C11—C10—H10 | 119.3 | C11′—C10′—H10′ | 119.8 |
| C6—C11—H11 | 120.4 | C6′—C11′—H11′ | 120.0 |
| C10—C11—C6 | 119.26 (12) | C10′—C11′—C6′ | 119.91 (13) |
| C10—C11—H11 | 120.4 | C10′—C11′—H11′ | 120.0 |
| C8—C12—H12A | 109.5 | C8′—C12′—H12D | 109.5 |
| C8—C12—H12B | 109.5 | C8′—C12′—H12E | 109.5 |
| C8—C12—H12C | 109.5 | C8′—C12′—H12F | 109.5 |
| H12A—C12—H12B | 109.5 | H12D—C12′—H12E | 109.5 |
| H12A—C12—H12C | 109.5 | H12D—C12′—H12F | 109.5 |
| H12B—C12—H12C | 109.5 | H12E—C12′—H12F | 109.5 |
| N4—C13—H13A | 110.0 | N4′—C13′—H13C | 109.9 |
| N4—C13—H13B | 110.0 | N4′—C13′—H13D | 109.9 |
| N4—C13—C14 | 108.63 (11) | N4′—C13′—C14′ | 108.83 (11) |
| H13A—C13—H13B | 108.3 | H13C—C13′—H13D | 108.3 |
| C14—C13—H13A | 110.0 | C14′—C13′—H13C | 109.9 |
| C14—C13—H13B | 110.0 | C14′—C13′—H13D | 109.9 |
| O2—C14—C13 | 112.48 (12) | O2′—C14′—C13′ | 112.23 (13) |
| O2—C14—H14A | 109.1 | O2′—C14′—H14C | 109.2 |
| O2—C14—H14B | 109.1 | O2′—C14′—H14D | 109.2 |
| C13—C14—H14A | 109.1 | C13′—C14′—H14C | 109.2 |
| C13—C14—H14B | 109.1 | C13′—C14′—H14D | 109.2 |
| H14A—C14—H14B | 107.8 | H14C—C14′—H14D | 107.9 |
| N4—C15—H15A | 109.6 | N4′—C15′—H15C | 109.8 |
| N4—C15—H15B | 109.6 | N4′—C15′—H15D | 109.8 |
| N4—C15—C16 | 110.33 (12) | N4′—C15′—C16′ | 109.59 (12) |
| H15A—C15—H15B | 108.1 | H15C—C15′—H15D | 108.2 |
| C16—C15—H15A | 109.6 | C16′—C15′—H15C | 109.8 |
| C16—C15—H15B | 109.6 | C16′—C15′—H15D | 109.8 |
| O2—C16—C15 | 111.14 (11) | O2′—C16′—C15′ | 111.32 (12) |
| O2—C16—H16A | 109.4 | O2′—C16′—H16C | 109.4 |
| O2—C16—H16B | 109.4 | O2′—C16′—H16D | 109.4 |
| C15—C16—H16A | 109.4 | C15′—C16′—H16C | 109.4 |
| C15—C16—H16B | 109.4 | C15′—C16′—H16D | 109.4 |
| H16A—C16—H16B | 108.0 | H16C—C16′—H16D | 108.0 |
| O1—C17—H17A | 110.4 | O1′—C17′—H17C | 109.3 |
| O1—C17—H17B | 110.4 | O1′—C17′—H17D | 109.3 |
| O1—C17—C18 | 106.76 (10) | O1′—C17′—C18′ | 111.53 (11) |
| H17A—C17—H17B | 108.6 | H17C—C17′—H17D | 108.0 |
| C18—C17—H17A | 110.4 | C18′—C17′—H17C | 109.3 |
| C18—C17—H17B | 110.4 | C18′—C17′—H17D | 109.3 |

| | | | |
|---|---|---|---|
| C17—C18—H18A | 109.7 | C17′—C18′—H18C | 109.5 |
| C17—C18—H18B | 109.7 | C17′—C18′—H18D | 109.5 |
| H18A—C18—H18B | 108.2 | H18C—C18′—H18D | 108.0 |
| C19—C18—C17 | 109.76 (11) | C19′—C18′—C17′ | 110.93 (11) |
| C19—C18—H18A | 109.7 | C19′—C18′—H18C | 109.5 |
| C19—C18—H18B | 109.7 | C19′—C18′—H18D | 109.5 |
| N6—C19—C18 | 115.92 (12) | N6′—C19′—C18′ | 116.42 (12) |
| N6—C19—C20 | 122.47 (13) | N6′—C19′—C20′ | 121.94 (13) |
| C20—C19—C18 | 121.57 (13) | C20′—C19′—C18′ | 121.62 (12) |
| C19—C20—H20 | 120.4 | C19′—C20′—H20′ | 120.2 |
| C19—C20—C21 | 119.29 (15) | C21′—C20′—C19′ | 119.64 (14) |
| C21—C20—H20 | 120.4 | C21′—C20′—H20′ | 120.2 |
| C20—C21—H21 | 120.6 | C20′—C21′—H21′ | 120.6 |
| C22—C21—C20 | 118.82 (15) | C22′—C21′—C20′ | 118.70 (14) |
| C22—C21—H21 | 120.6 | C22′—C21′—H21′ | 120.6 |
| C21—C22—H22 | 120.7 | C21′—C22′—H22′ | 120.9 |
| C21—C22—C23 | 118.60 (14) | C21′—C22′—C23′ | 118.23 (14) |
| C23—C22—H22 | 120.7 | C23′—C22′—H22′ | 120.9 |
| N6—C23—C22 | 123.52 (15) | N6′—C23′—C22′ | 124.28 (14) |
| N6—C23—H23 | 118.2 | N6′—C23′—H23′ | 117.9 |
| C22—C23—H23 | 118.2 | C22′—C23′—H23′ | 117.9 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···N2′ | 0.91 (1) | 2.16 (1) | 3.0626 (16) | 169 (1) |
| N1′—H1′···N2 | 0.92 (1) | 2.10 (1) | 3.0129 (16) | 178 (2) |