IUCrData

ISSN 2414-3146

1-Cyclohexyl-5-(2-hydroxybenzoyl)-3-nitropyridin-2(1*H*)-one

T. Siva Ranjani,[a] N. Poomathi,[b] G. Vimala,[a] Paramasivam T. Perumal[b] and K. Sakthi Murugesan[a]*

[a]Department of Physics, Presidency College (Autonomous), Chennai 600 005, India, and [b]Organic Chemistry Division, Central Leather Research Institute, Adyar, Chennai 602 020, India. *Correspondence e-mail: ksakthimurugesan2492@gmail.com

Received 28 November 2016
Accepted 3 January 2017

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

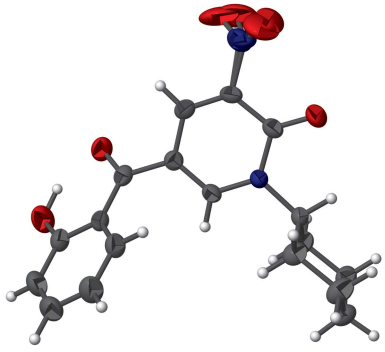
Keywords: crystal structure; nitropyridine derivatives; hydrogen bonding; C—H–π interactions..

CCDC reference: 1525355

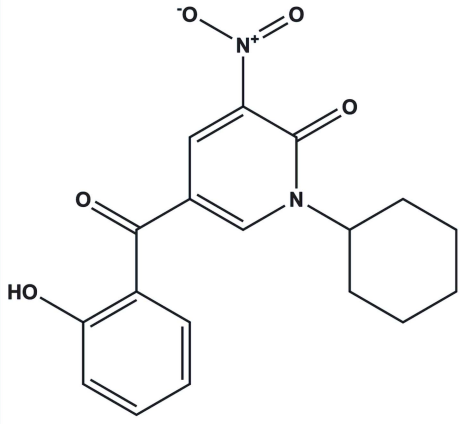
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{18}H_{18}N_2O_5$, the cyclohexane ring adopts a chair conformation, and its mean plane is almost normal to the central pyridin-2-one ring with a dihedral angle of 87.94 (8)°. The latter ring is inclined to the 2-hydroxybenzoyl ring by 50.92 (8)°. There is an intramolecular O—H···O hydrogen bond in this unit forming an *S*(6) ring motif. The NO_2 group is disordered over two orientations of equal occupancy. In the crystal, molecules are linked *via* C—H···O hydrogen bonds, forming chains propagating along [001]. Inversion-related chains are linked by C—H···π interactions, forming columns along the *c*-axis direction.

3D view



Chemical scheme



Structure description

The title nitropyridine compound is widely used in the synthesis of heterocyclic drugs and cytokine inhibitors (Hu *et al.*, 2011). Studies of pyridine and pyrimidine derivatives, related to the title compound, are also of interest owing to their properties, such as fluorescence (Kawai *et al.* 2001; Abdullah, 2005).

In the title compound, Fig. 1, the cyclohexane ring (C13–C18) adopts a chair conformation [puckering parameters: Q = 0.57 (18) Å and φ_2 = 178.34 (18) °]. Its mean plane is almost normal to the central pyridin-2-one ring (N1/C1–C5), making a dihedral angle of 87.94 (8)°. The latter ring is inclined to the 2-hydroxybenzoyl ring (C7–C12) by 50.92 (8)°. There is an intramolecular O—H···O hydrogen bond in this unit forming an *S*(6) ring motif (Table 1 and Fig. 1). The nitro group is disordered over two orientations and inclined to the pyridine ring to which it is attached by 40 (3) and 61 (4) ° for planes N1/O1/O2 and N1′/O1′/O2′, respectively. The geometrical parameters of the title compound are close to those observed for a similar nitropyridine compound,

OPEN ACCESS

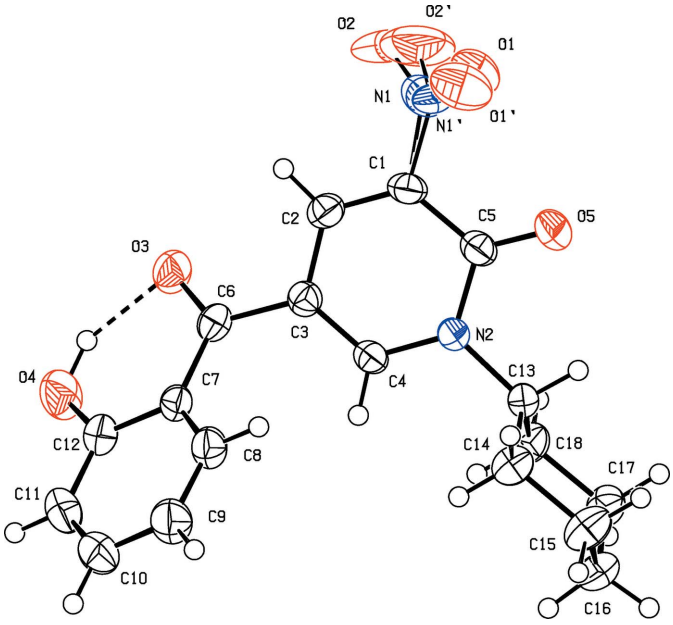


Figure 1
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular O—H···O hydrogen bond is shown as a dashed line (see Table 1).

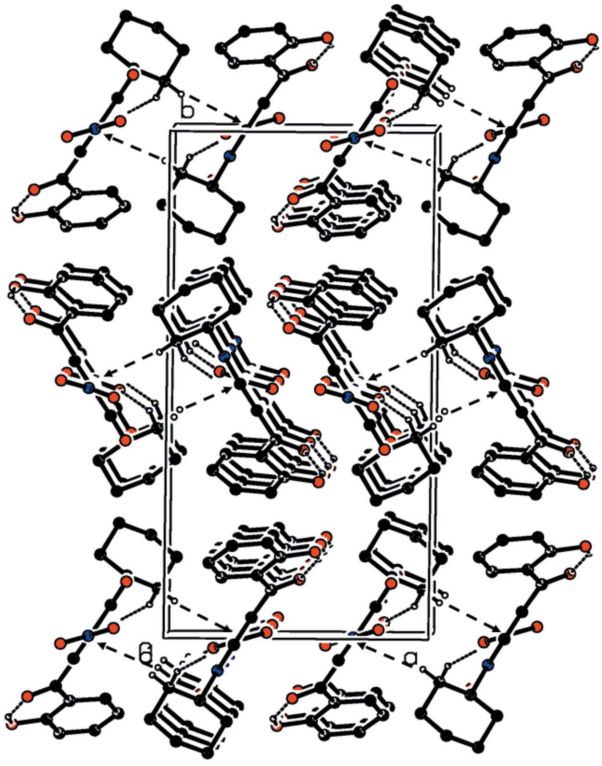


Figure 2
A view along the *c* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines and the C—H···π interactions are represented by dashed arrows (see Table 1). For clarity, only H atoms H4*A*, H14*A* and H14*B*, and one component of the disordered NO_2 group, have been included.

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

*Cg*1 is the centroid of the N1/C1–C5 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O3	0.94 (2)	1.78 (2)	2.602 (2)	146 (2)
C14—H14*A*···O1^{i}	0.97	2.44	3.341 (19)	155
C14—H14*A*···O1$'^{i}$	0.97	2.57	3.508 (19)	163
C14—H14*B*···*Cg*1^{ii}	0.97	2.87	3.596 (2)	132

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{18}N_2O_5$
M_r	342.34
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, *b*, *c* (Å)	10.1622 (6), 19.1448 (8), 8.4373 (5)
β (°)	102.425 (3)
V (Å^3)	1603.06 (15)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.35 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.964, 0.979
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22797, 2813, 2106
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.036, 0.094, 1.04
No. of reflections	2813
No. of parameters	258
No. of restraints	79
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.14

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

5-(2-hydroxybenzoyl)-1-methyl-3-nitropyridin-2(1*H*)-one (Vimala *et al.*, 2016).

In the crystal, molecules are linked *via* C—H···O hydrogen bonds, forming chains propagating along [001]; see Table 1 and Fig. 2. Inversion-related chains are linked by C—H···π interactions (Table 1), forming columns along the *c*-axis direction, as shown in Fig. 2.

Synthesis and crystallization

A mixture of 3-formylchromone (1 mmol), (*Z*)-*N*-(1-(methylthio)-2-nitrovinyl)cyclohexanamine (1 mmol), and indium trifluoromethanesulfonate (0.020 mmol) in ethanol (3 mmol) were charged in a 25 ml round-bottomed flask and

the mixture was heated at reflux. The resulting solution was stirred for 1 h during reflux. After completion of the reaction, monitored by TLC, the product was filtered and washed with ethanol, and dried under vacuum to obtain the product in 87% yield. It was recrystallized from a solution in ethanol:DMSO-D6 (1:1) by slow evaporation of the solvents, and gave yellow plate-like crystals suitable for X-ray diffraction analysis.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The NO_2 group is disordered over two positions (N1/O1/O2:N1′/O1′/O2′) with an occupancy ratio 0.50 (2):0.50 (2).

Acknowledgements

The authors thank Dr Babu Varghese, SAIF, IIT, Chennai, India, for the data collection.

References

Abdullah, Z. (2005). *Int. J. Chem. Sci.* **3**, 9–15.
Bruker (2008). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hu, Y., Jin, Y. Z., Xiong, Y. P. & Li, Z. C. (2011). *Sci. Technol. Eng.* **11**, 1841–1843.
Kawai, M., Lee, M. J., Evans, K. O. & Nordlund, T. M. (2001). *J. Fluoresc.* **11**, 23–32.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Vimala, G., Poomathi, N., Perumal, P. T. & SubbiahPandi, A. (2016). 1, x160527.

full crystallographic data

IUCrData (2017). **2**, x170004 [https://doi.org/10.1107/S2414314617000049]

1-Cyclohexyl-5-(2-hydroxybenzoyl)-3-nitropyridin-2(1*H*)-one

T. Siva Ranjani, N. Poomathi, G. Vimala, Paramasivam T. Perumal and K. Sakthi Murugesan

1-Cyclohexyl-5-(2-hydroxycyclohexanecarbonyl)-3-nitropyridin-2(1H)-one

Crystal data

$C_{18}H_{18}N_2O_5$
M_r = 342.34
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 10.1622 (6) Å
b = 19.1448 (8) Å
c = 8.4373 (5) Å
β = 102.425 (3)°
V = 1603.06 (15) Å^3
Z = 4
$F(000)$ = 720
D_x = 1.418 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2106 reflections
θ = 2.3–25.0°
μ = 0.11 mm^{-1}
T = 293 K
Plate, yellow
0.35 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.964, T_{max} = 0.979
22797 measured reflections
2813 independent reflections
2106 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −12→12
k = −22→22
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 1.04
2813 reflections
258 parameters
79 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 0.4118P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 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. 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.72235 (17)	0.00339 (8)	0.72648 (18)	0.0350 (4)	
C2	0.65445 (17)	−0.04697 (8)	0.63265 (19)	0.0341 (4)	
H2	0.6056	−0.0800	0.6768	0.041*	
C3	0.65766 (16)	−0.04945 (8)	0.46653 (18)	0.0305 (4)	
C4	0.72131 (16)	0.00358 (7)	0.40569 (18)	0.0297 (4)	
H4	0.7216	0.0035	0.2955	0.036*	
C5	0.79293 (17)	0.05961 (8)	0.66724 (18)	0.0338 (4)	
C6	0.58259 (16)	−0.10552 (8)	0.36459 (19)	0.0316 (4)	
C7	0.63282 (16)	−0.13627 (7)	0.22978 (18)	0.0312 (4)	
C8	0.76772 (17)	−0.13196 (8)	0.2183 (2)	0.0387 (4)	
H8	0.8280	−0.1076	0.2975	0.046*	
C9	0.8138 (2)	−0.16251 (9)	0.0941 (2)	0.0484 (5)	
H9	0.9043	−0.1595	0.0897	0.058*	
C10	0.7237 (2)	−0.19801 (9)	−0.0249 (2)	0.0518 (5)	
H10	0.7535	−0.2180	−0.1113	0.062*	
C11	0.5909 (2)	−0.20406 (10)	−0.0171 (2)	0.0507 (5)	
H11	0.5314	−0.2280	−0.0981	0.061*	
C12	0.54465 (18)	−0.17466 (8)	0.1108 (2)	0.0379 (4)	
C13	0.84628 (16)	0.11433 (7)	0.42306 (18)	0.0313 (4)	
H13	0.8831	0.1475	0.5098	0.038*	
C14	0.96297 (17)	0.08852 (8)	0.3544 (2)	0.0379 (4)	
H14A	0.9307	0.0553	0.2679	0.045*	
H14B	1.0278	0.0649	0.4386	0.045*	
C15	1.03031 (19)	0.14974 (10)	0.2888 (2)	0.0493 (5)	
H15A	1.0715	0.1800	0.3779	0.059*	
H15B	1.1010	0.1324	0.2381	0.059*	
C16	0.92978 (19)	0.19132 (9)	0.1659 (2)	0.0451 (5)	
H16A	0.9744	0.2319	0.1328	0.054*	
H16B	0.8975	0.1628	0.0705	0.054*	
C17	0.81130 (18)	0.21494 (8)	0.2339 (2)	0.0402 (4)	
H17A	0.7465	0.2385	0.1496	0.048*	
H17B	0.8420	0.2481	0.3210	0.048*	
C18	0.74314 (17)	0.15355 (8)	0.2984 (2)	0.0382 (4)	
H18A	0.6713	0.1704	0.3477	0.046*	
H18B	0.7041	0.1226	0.2098	0.046*	
O3	0.47702 (12)	−0.12623 (6)	0.39842 (15)	0.0448 (3)	
O4	0.41388 (13)	−0.18460 (7)	0.11370 (18)	0.0573 (4)	
O5	0.85183 (15)	0.10691 (6)	0.74796 (14)	0.0550 (4)	
N2	0.78391 (13)	0.05618 (6)	0.49840 (14)	0.0288 (3)	
N1	0.714 (2)	0.0019 (12)	0.8973 (13)	0.058 (4)	0.50 (6)

O1	0.811 (3)	0.0188 (13)	0.9989 (19)	0.091 (4)	0.50 (6)
O2	0.610 (2)	−0.0133 (15)	0.932 (2)	0.094 (4)	0.50 (6)
N1′	0.733 (2)	0.0058 (13)	0.9032 (12)	0.054 (3)	0.50 (6)
O1′	0.847 (2)	0.0006 (14)	0.986 (2)	0.089 (4)	0.50 (6)
O2′	0.630 (3)	0.0080 (17)	0.949 (2)	0.107 (5)	0.50 (6)
H4A	0.402 (2)	−0.1694 (13)	0.215 (3)	0.089 (8)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0481 (11)	0.0341 (9)	0.0249 (8)	0.0055 (8)	0.0123 (7)	0.0017 (7)
C2	0.0387 (10)	0.0296 (8)	0.0372 (9)	0.0021 (7)	0.0152 (8)	0.0034 (7)
C3	0.0308 (9)	0.0288 (8)	0.0323 (8)	0.0009 (7)	0.0078 (7)	−0.0008 (6)
C4	0.0340 (9)	0.0297 (8)	0.0255 (8)	0.0016 (7)	0.0065 (7)	−0.0028 (6)
C5	0.0413 (10)	0.0327 (9)	0.0265 (8)	0.0023 (7)	0.0053 (7)	−0.0027 (7)
C6	0.0299 (9)	0.0277 (8)	0.0365 (9)	−0.0001 (7)	0.0056 (7)	0.0047 (7)
C7	0.0347 (9)	0.0252 (8)	0.0334 (8)	−0.0026 (7)	0.0069 (7)	0.0002 (6)
C8	0.0361 (10)	0.0356 (9)	0.0440 (10)	−0.0048 (8)	0.0080 (8)	−0.0055 (8)
C9	0.0432 (11)	0.0475 (10)	0.0588 (12)	−0.0029 (9)	0.0206 (10)	−0.0105 (9)
C10	0.0632 (14)	0.0463 (10)	0.0511 (11)	−0.0047 (10)	0.0243 (10)	−0.0145 (9)
C11	0.0580 (13)	0.0470 (10)	0.0465 (11)	−0.0122 (9)	0.0101 (10)	−0.0158 (9)
C12	0.0382 (10)	0.0330 (9)	0.0422 (10)	−0.0070 (8)	0.0079 (8)	−0.0020 (7)
C13	0.0396 (9)	0.0262 (8)	0.0282 (8)	−0.0057 (7)	0.0070 (7)	−0.0023 (6)
C14	0.0338 (10)	0.0387 (9)	0.0412 (9)	0.0037 (7)	0.0078 (8)	0.0072 (7)
C15	0.0395 (11)	0.0505 (11)	0.0605 (12)	0.0002 (9)	0.0166 (9)	0.0141 (9)
C16	0.0530 (12)	0.0414 (10)	0.0430 (10)	−0.0037 (8)	0.0151 (9)	0.0109 (8)
C17	0.0461 (11)	0.0321 (9)	0.0404 (10)	0.0014 (8)	0.0048 (8)	0.0066 (7)
C18	0.0368 (10)	0.0326 (8)	0.0464 (10)	0.0038 (7)	0.0113 (8)	0.0049 (7)
O3	0.0384 (7)	0.0443 (7)	0.0549 (8)	−0.0096 (6)	0.0176 (6)	−0.0064 (6)
O4	0.0422 (8)	0.0688 (9)	0.0605 (9)	−0.0197 (7)	0.0101 (7)	−0.0198 (7)
O5	0.0845 (10)	0.0465 (7)	0.0317 (7)	−0.0202 (7)	0.0076 (6)	−0.0087 (6)
N2	0.0350 (8)	0.0259 (6)	0.0254 (7)	−0.0018 (6)	0.0063 (6)	−0.0013 (5)
N1	0.096 (7)	0.039 (6)	0.039 (6)	0.004 (6)	0.017 (4)	−0.003 (4)
O1	0.145 (10)	0.089 (7)	0.035 (3)	−0.043 (6)	0.009 (5)	−0.012 (4)
O2	0.117 (6)	0.124 (10)	0.060 (5)	0.001 (6)	0.058 (4)	0.022 (5)
N1′	0.098 (7)	0.042 (5)	0.029 (5)	−0.016 (5)	0.028 (4)	0.002 (4)
O1′	0.120 (7)	0.109 (8)	0.029 (4)	−0.013 (6)	−0.006 (4)	0.003 (4)
O2′	0.136 (9)	0.128 (10)	0.080 (5)	0.014 (6)	0.078 (6)	−0.001 (6)

Geometric parameters (Å, º)

C1—C2	1.341 (2)	C12—O4	1.348 (2)
C1—C5	1.441 (2)	C13—N2	1.4895 (19)
C1—N1	1.463 (10)	C13—C14	1.511 (2)
C1—N1′	1.472 (9)	C13—C18	1.515 (2)
C2—C3	1.410 (2)	C13—H13	0.9800
C2—H2	0.9300	C14—C15	1.520 (2)
C3—C4	1.362 (2)	C14—H14A	0.9700

C3—C6	1.480 (2)	C14—H14B	0.9700
C4—N2	1.3477 (18)	C15—C16	1.516 (2)
C4—H4	0.9300	C15—H15A	0.9700
C5—O5	1.2111 (19)	C15—H15B	0.9700
C5—N2	1.4092 (19)	C16—C17	1.510 (2)
C6—O3	1.2335 (18)	C16—H16A	0.9700
C6—C7	1.467 (2)	C16—H16B	0.9700
C7—C8	1.397 (2)	C17—C18	1.523 (2)
C7—C12	1.401 (2)	C17—H17A	0.9700
C8—C9	1.368 (2)	C17—H17B	0.9700
C8—H8	0.9300	C18—H18A	0.9700
C9—C10	1.383 (3)	C18—H18B	0.9700
C9—H9	0.9300	O4—H4A	0.94 (3)
C10—C11	1.370 (3)	N1—O2	1.193 (11)
C10—H10	0.9300	N1—O1	1.209 (11)
C11—C12	1.386 (2)	N1′—O2′	1.196 (11)
C11—H11	0.9300	N1′—O1′	1.216 (12)

C2—C1—C5	124.31 (14)	C14—C13—H13	107.1
C2—C1—N1	115.8 (10)	C18—C13—H13	107.1
C5—C1—N1	119.8 (10)	C13—C14—C15	109.83 (13)
C2—C1—N1′	122.6 (9)	C13—C14—H14A	109.7
C5—C1—N1′	113.1 (9)	C15—C14—H14A	109.7
N1—C1—N1′	8.2 (14)	C13—C14—H14B	109.7
C1—C2—C3	119.49 (15)	C15—C14—H14B	109.7
C1—C2—H2	120.3	H14A—C14—H14B	108.2
C3—C2—H2	120.3	C16—C15—C14	111.35 (15)
C4—C3—C2	117.64 (14)	C16—C15—H15A	109.4
C4—C3—C6	123.27 (14)	C14—C15—H15A	109.4
C2—C3—C6	118.87 (14)	C16—C15—H15B	109.4
N2—C4—C3	122.77 (14)	C14—C15—H15B	109.4
N2—C4—H4	118.6	H15A—C15—H15B	108.0
C3—C4—H4	118.6	C17—C16—C15	111.86 (14)
O5—C5—N2	121.33 (15)	C17—C16—H16A	109.2
O5—C5—C1	125.88 (14)	C15—C16—H16A	109.2
N2—C5—C1	112.76 (13)	C17—C16—H16B	109.2
O3—C6—C7	121.04 (14)	C15—C16—H16B	109.2
O3—C6—C3	117.63 (14)	H16A—C16—H16B	107.9
C7—C6—C3	121.32 (14)	C16—C17—C18	111.46 (14)
C8—C7—C12	117.84 (15)	C16—C17—H17A	109.3
C8—C7—C6	122.72 (14)	C18—C17—H17A	109.3
C12—C7—C6	119.36 (15)	C16—C17—H17B	109.3
C9—C8—C7	122.06 (16)	C18—C17—H17B	109.3
C9—C8—H8	119.0	H17A—C17—H17B	108.0
C7—C8—H8	119.0	C13—C18—C17	109.31 (14)
C8—C9—C10	118.91 (18)	C13—C18—H18A	109.8
C8—C9—H9	120.5	C17—C18—H18A	109.8
C10—C9—H9	120.5	C13—C18—H18B	109.8

C11—C10—C9	120.80 (17)	C17—C18—H18B	109.8
C11—C10—H10	119.6	H18A—C18—H18B	108.3
C9—C10—H10	119.6	C12—O4—H4A	107.1 (15)
C10—C11—C12	120.38 (17)	C4—N2—C5	122.78 (13)
C10—C11—H11	119.8	C4—N2—C13	120.12 (12)
C12—C11—H11	119.8	C5—N2—C13	117.10 (12)
O4—C12—C11	117.22 (16)	O2—N1—O1	122.0 (14)
O4—C12—C7	122.84 (15)	O2—N1—C1	119.3 (14)
C11—C12—C7	119.94 (16)	O1—N1—C1	118.6 (15)
N2—C13—C14	111.12 (12)	O2′—N1′—O1′	127.2 (15)
N2—C13—C18	111.87 (13)	O2′—N1′—C1	116.7 (14)
C14—C13—C18	112.26 (13)	O1′—N1′—C1	116.0 (14)
N2—C13—H13	107.1		

C5—C1—C2—C3	4.5 (3)	C6—C7—C12—C11	−179.93 (15)
N1—C1—C2—C3	−179.8 (9)	N2—C13—C14—C15	−176.16 (13)
N1′—C1—C2—C3	−174.6 (10)	C18—C13—C14—C15	57.71 (18)
C1—C2—C3—C4	−5.4 (2)	C13—C14—C15—C16	−55.0 (2)
C1—C2—C3—C6	179.78 (14)	C14—C15—C16—C17	54.6 (2)
C2—C3—C4—N2	2.2 (2)	C15—C16—C17—C18	−55.1 (2)
C6—C3—C4—N2	176.74 (14)	N2—C13—C18—C17	176.42 (13)
C2—C1—C5—O5	177.75 (17)	C14—C13—C18—C17	−57.85 (17)
N1—C1—C5—O5	2.3 (9)	C16—C17—C18—C13	55.73 (18)
N1′—C1—C5—O5	−3.1 (9)	C3—C4—N2—C5	2.2 (2)
C2—C1—C5—N2	−0.3 (2)	C3—C4—N2—C13	−177.20 (14)
N1—C1—C5—N2	−175.7 (9)	O5—C5—N2—C4	178.73 (15)
N1′—C1—C5—N2	178.9 (9)	C1—C5—N2—C4	−3.1 (2)
C4—C3—C6—O3	−141.48 (16)	O5—C5—N2—C13	−1.8 (2)
C2—C3—C6—O3	33.0 (2)	C1—C5—N2—C13	176.31 (13)
C4—C3—C6—C7	39.5 (2)	C14—C13—N2—C4	−65.36 (18)
C2—C3—C6—C7	−145.97 (15)	C18—C13—N2—C4	60.99 (18)
O3—C6—C7—C8	−158.65 (15)	C14—C13—N2—C5	115.17 (15)
C3—C6—C7—C8	20.3 (2)	C18—C13—N2—C5	−118.48 (15)
O3—C6—C7—C12	18.1 (2)	C2—C1—N1—O2	−38 (2)
C3—C6—C7—C12	−162.94 (14)	C5—C1—N1—O2	137.5 (18)
C12—C7—C8—C9	1.4 (2)	N1′—C1—N1—O2	175 (14)
C6—C7—C8—C9	178.21 (15)	C2—C1—N1—O1	145 (2)
C7—C8—C9—C10	0.8 (3)	C5—C1—N1—O1	−40 (3)
C8—C9—C10—C11	−1.5 (3)	N1′—C1—N1—O1	−3 (11)
C9—C10—C11—C12	−0.1 (3)	C2—C1—N1′—O2′	−58 (3)
C10—C11—C12—O4	−177.84 (17)	C5—C1—N1′—O2′	123 (2)
C10—C11—C12—C7	2.4 (3)	N1—C1—N1′—O2′	−22 (11)
C8—C7—C12—O4	177.25 (15)	C2—C1—N1′—O1′	117 (2)
C6—C7—C12—O4	0.3 (2)	C5—C1—N1′—O1′	−62 (2)
C8—C7—C12—C11	−3.0 (2)	N1—C1—N1′—O1′	153 (14)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the N1/C1–C5 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O3	0.94 (2)	1.78 (2)	2.602 (2)	146 (2)
C14—H14*A*···O1^{i}	0.97	2.44	3.341 (19)	155
C14—H14*A*···O1′^{i}	0.97	2.57	3.508 (19)	163
C14—H14*B*···*Cg*1^{ii}	0.97	2.87	3.596 (2)	132

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