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(*E*)-*N*′-(2,3,4-Trimethoxybenzylidene)-isonicotinohydrazide

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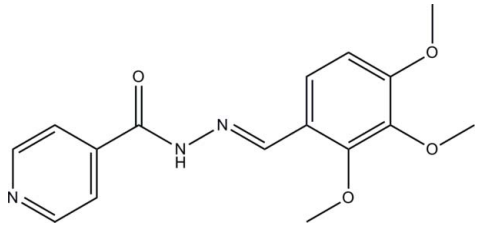
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.159; data-to-parameter ratio = 16.2.

In the title compound, $C_{16}H_{17}N_3O_4$, the molecule exists in an *E* configuration with respect to the C=N double bond. The molecule is not planar, the dihedral angle between the pyridine and benzene rings being 71.67 (8)°. In the crystal structure, molecules are linked into chains along the *b* axis by bifurcated N—H···O and C—H···O hydrogen bonds. These chains are linked into a three-dimensional network by C—H···O and C—H···π interactions.

Related literature

For applications of isoniazid derivatives, see: Janin (2007); Maccari *et al.* (2005); Slayden & Barry (2000); Kahwa *et al.* (1986). For preparation of the compound, see: Lourenco *et al.* (2008). For related structures, see: Naveenkumar *et al.* (2009, 2010*a*,*b*); Shi (2005). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{16}H_{17}N_3O_4$
M_r = 315.33
Monoclinic, $P2_1/c$
a = 14.246 (3) Å
b = 9.397 (2) Å
c = 12.098 (3) Å
β = 109.245 (6)°
V = 1529.1 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 K
0.38 × 0.33 × 0.14 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.963, T_{max} = 0.986
14341 measured reflections
3482 independent reflections
2988 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.159
S = 1.10
3482 reflections
215 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

*Cg*1 is the centroid of the C1/C2/N1/C3/C4/C5 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1*N*2···O1^{i}	0.91 (3)	2.09 (3)	2.7987 (19)	134 (2)
C4—H4*A*···O1^{i}	0.93	2.46	3.348 (2)	159
C14—H14*C*···O3	0.96	2.55	3.113 (2)	118
C15—H15*C*···O2^{ii}	0.96	2.49	3.292 (2)	141
C16—H16*A*···O3^{iii}	0.96	2.57	3.518 (2)	167
C14—H14*B*···*Cg*1^{i}	0.96	2.81	3.719 (3)	159

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

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: TK2657).

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§ Thomson Reuters ResearcherID: A-5523-2009.
¶ Thomson Reuters ResearcherID: A-3561-2009.

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supporting information

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(*E*)-*N*′-(2,3,4-Trimethoxybenzylidene)isonicotinohydrazide

H. S. Naveenkumar, Amirin Sadikun, Pazilah Ibrahim, Chin Sing Yeap and Hoong-Kun Fun

S1. Comment

In the search of new compounds of pharmaceutical importance, isoniazid derivatives have been found to possess potential tuberculostatic activity (Janin, 2007; Maccari *et al.*, 2005; Slayden & Barry, 2000). Schiff bases have attracted much attention because of their biological activity (Kahwa *et al.*, 1986). As a part of on-going work into the synthesis of (*E*)-*N*′-substituted isonicotinohydrazide derivatives, in this paper we present the crystal structure of the title compound (I).

The geometric parameters of (I) are comparable to those in related structures (Naveenkumar *et al.*, 2009, 2010a, 2010b; Shi, 2005). The molecule exists in an *E* configuration with respect to the C7═N3 double bond (Fig. 1). The isoniazid group is twisted away with the torsion angle of C1–C5–C6–N2 being -149.60 (15)°. The dihedral angle between the pyridine ring and the benzene ring is 71.67 (8)°. One of the methoxy group is coplanar with the benzene ring whereas the other two are twisted away from the benzene ring [torsion angles: C16–O4–C11–C12 = -3.8 (2), C15–O3–C10–C11 = -97.83 (17), C14–O2–C9–C10 = 73.23 (19) °]. A weak intramolecular C14–H14C···O3 hydrogen bond stabilizes the molecular structure (Table 1). In the crystal structure, the molecules are linked into one-dimensional chains along the *b* axis by the bifurcated intermolecular N2–H1N2···O1 and C4–H4A···O1 hydrogen bonds (Table 1). These chains are linked into a three-dimensional network by C15–H15C···O2, C16–H16A···O3 and C14–H14B···*Cg*1 interactions (Fig. 2, Table 1).

S2. Experimental

The isoniazid derivative (I) was prepared following the procedure by Lourenco *et al.* (2008). 2,3,4-Trimethoxybenzaldehyde (1.0 eq) was reacted with isoniazid (1.0 eq) in ethanol/water. After stirring for 3 h at room temperature, the resulting mixture was concentrated under reduced pressure. The residue was purified by washing with cold ethanol and ethyl ether, affording the pure derivative. The colourless crystals were obtained by recrystallization from a methanol solution of (I).

S3. Refinement

The H1N2 H atom was located from a difference Fourier map and refined freely. The remaining H atoms were positioned geometrically [C–H = 0.93 or 0.96 Å] and refined using a riding model, with U_{iso}(H) = 1.2 or 1.5 U_{eq}(C). A rotating-group model was applied for the methyl groups.

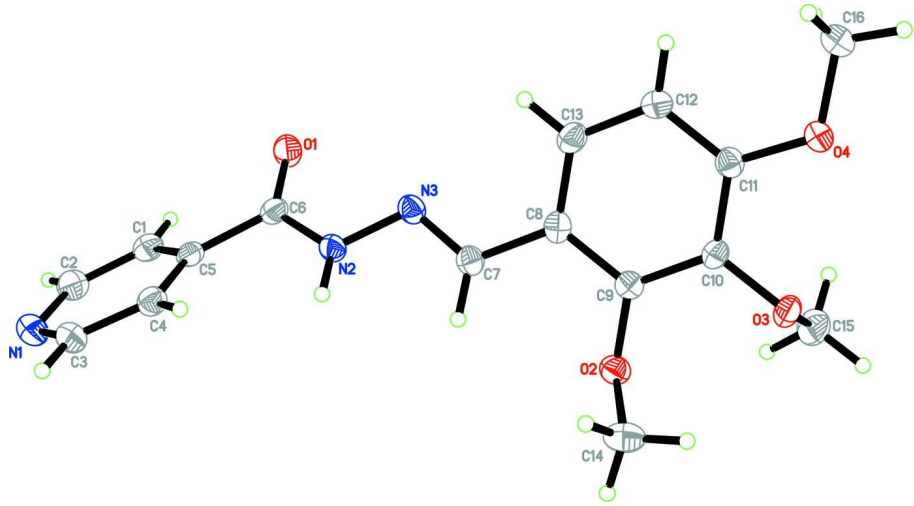

Figure 1

The molecular structure of (I) with atom labels and 50% probability ellipsoids for non-H atoms.

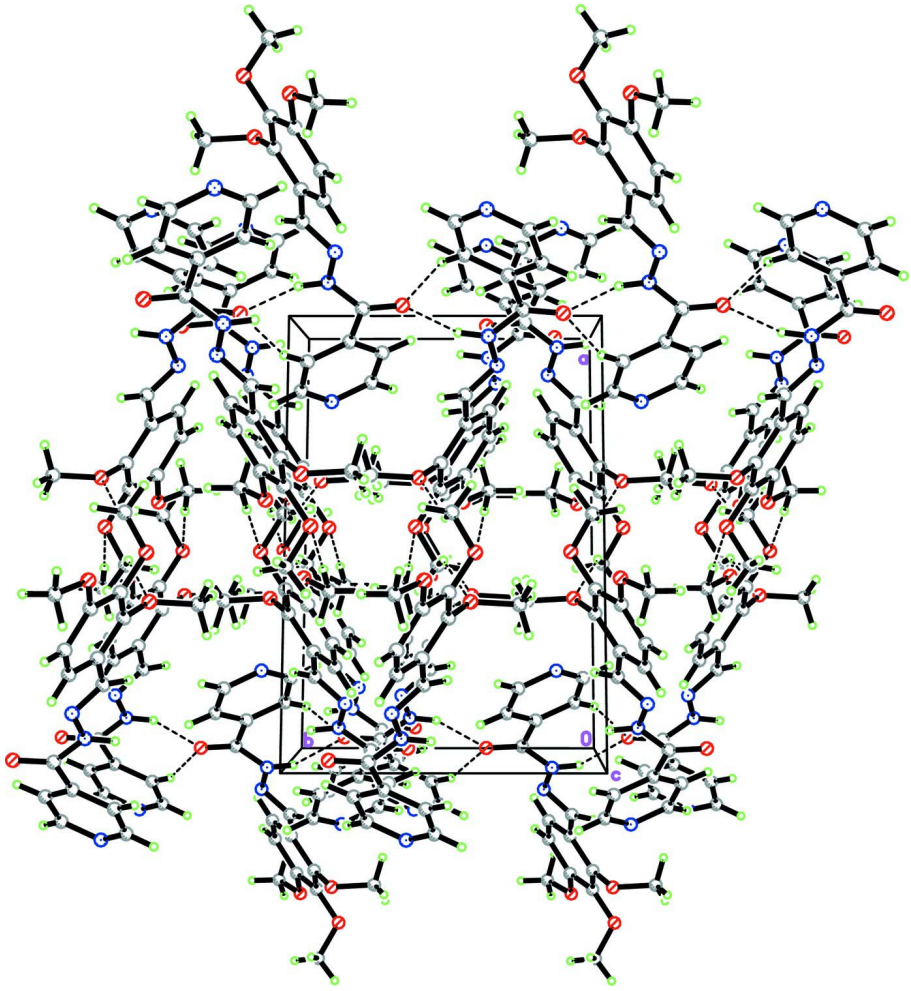

Figure 2

The crystal packing of (I), viewed down the *c* axis, showing the molecules are linked into a 3-D network. Intermolecular contacts are shown as dashed lines.

(*E*)-*N*′-(2,3,4-Trimethoxybenzylidene)isonicotinohydrazide

Crystal data

$C_{16}H_{17}N_3O_4$
$M_r = 315.33$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.246\ (3)$ Å
$b = 9.397\ (2)$ Å
$c = 12.098\ (3)$ Å
$\beta = 109.245\ (6)°$
$V = 1529.1\ (6)$ Å^3
$Z = 4$

$F(000) = 664$
$D_x = 1.370$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5847 reflections
$\theta = 2.8–33.0°$
$\mu = 0.10$ mm^{-1}
$T = 100$ K
Block, colourless
0.38 × 0.33 × 0.14 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.963, T_{max} = 0.986
14341 measured reflections
3482 independent reflections
2988 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 27.5°, θ_{min} = 2.6°
h = −17→18
k = −11→12
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.159
S = 1.10
3482 reflections
215 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0903P)^2 + 0.7464P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.01090 (9)	0.86823 (12)	−0.28320 (11)	0.0286 (3)
O2	0.36424 (9)	0.41851 (12)	−0.00731 (10)	0.0232 (3)
O3	0.47223 (8)	0.40332 (13)	0.23303 (10)	0.0235 (3)
O4	0.41436 (9)	0.55428 (13)	0.38640 (10)	0.0245 (3)
N1	−0.18863 (12)	0.63126 (17)	−0.66119 (13)	0.0302 (4)
N2	0.05989 (10)	0.63755 (14)	−0.24901 (12)	0.0207 (3)
N3	0.11895 (10)	0.66421 (14)	−0.13400 (11)	0.0208 (3)
C1	−0.08316 (12)	0.79807 (18)	−0.52380 (15)	0.0238 (3)
H1A	−0.0557	0.8888	−0.5098	0.029*
C2	−0.14580 (13)	0.76010 (19)	−0.63502 (15)	0.0277 (4)
H2A	−0.1587	0.8275	−0.6944	0.033*
C3	−0.16847 (13)	0.53782 (19)	−0.57329 (15)	0.0278 (4)
H3A	−0.1983	0.4487	−0.5894	0.033*
C4	−0.10626 (12)	0.56370 (17)	−0.45947 (15)	0.0231 (3)

H4A	−0.0942	0.4937	−0.4021	0.028*
C5	−0.06239 (11)	0.69824 (17)	−0.43404 (14)	0.0204 (3)
C6	0.00512 (11)	0.74314 (16)	−0.31422 (14)	0.0203 (3)
C7	0.18304 (11)	0.56473 (17)	−0.09093 (13)	0.0200 (3)
H7A	0.1910	0.4914	−0.1387	0.024*
C8	0.24315 (11)	0.56734 (16)	0.03316 (14)	0.0198 (3)
C9	0.33100 (11)	0.48599 (16)	0.07346 (13)	0.0184 (3)
C10	0.38660 (11)	0.48299 (16)	0.19251 (13)	0.0188 (3)
C11	0.35435 (12)	0.56152 (17)	0.27246 (14)	0.0205 (3)
C12	0.26610 (12)	0.63962 (17)	0.23309 (15)	0.0233 (3)
H12A	0.2438	0.6895	0.2860	0.028*
C13	0.21207 (12)	0.64218 (17)	0.11454 (14)	0.0229 (3)
H13A	0.1537	0.6951	0.0886	0.027*
C14	0.35843 (15)	0.26623 (19)	−0.00823 (17)	0.0325 (4)
H14A	0.3768	0.2297	−0.0723	0.049*
H14B	0.2917	0.2376	−0.0171	0.049*
H14C	0.4029	0.2294	0.0641	0.049*
C15	0.55771 (13)	0.4749 (2)	0.22131 (17)	0.0324 (4)
H15A	0.6152	0.4152	0.2516	0.049*
H15B	0.5682	0.5626	0.2644	0.049*
H15C	0.5468	0.4945	0.1401	0.049*
C16	0.38727 (14)	0.6398 (2)	0.46951 (15)	0.0308 (4)
H16A	0.4343	0.6248	0.5463	0.046*
H16B	0.3221	0.6132	0.4690	0.046*
H16C	0.3873	0.7384	0.4488	0.046*
H1N2	0.0529 (18)	0.544 (3)	−0.270 (2)	0.038 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0297 (6)	0.0180 (6)	0.0300 (6)	0.0029 (5)	−0.0011 (5)	−0.0029 (5)
O2	0.0270 (6)	0.0225 (6)	0.0204 (6)	0.0008 (4)	0.0083 (5)	−0.0008 (4)
O3	0.0192 (6)	0.0264 (6)	0.0232 (6)	0.0059 (4)	0.0047 (4)	0.0030 (4)
O4	0.0264 (6)	0.0278 (6)	0.0176 (6)	0.0044 (5)	0.0048 (5)	−0.0011 (4)
N1	0.0324 (8)	0.0321 (8)	0.0239 (7)	0.0010 (6)	0.0062 (6)	−0.0048 (6)
N2	0.0224 (7)	0.0167 (6)	0.0202 (6)	0.0005 (5)	0.0032 (5)	−0.0022 (5)
N3	0.0217 (6)	0.0189 (6)	0.0200 (6)	−0.0027 (5)	0.0045 (5)	−0.0024 (5)
C1	0.0234 (7)	0.0205 (8)	0.0288 (8)	0.0018 (6)	0.0104 (6)	0.0013 (6)
C2	0.0306 (9)	0.0289 (9)	0.0244 (8)	0.0040 (7)	0.0101 (7)	0.0026 (6)
C3	0.0276 (8)	0.0244 (8)	0.0285 (8)	−0.0007 (7)	0.0055 (7)	−0.0062 (7)
C4	0.0214 (7)	0.0200 (8)	0.0272 (8)	0.0014 (6)	0.0071 (6)	0.0000 (6)
C5	0.0181 (7)	0.0197 (7)	0.0243 (8)	0.0031 (6)	0.0080 (6)	−0.0013 (6)
C6	0.0178 (7)	0.0172 (7)	0.0257 (8)	0.0011 (6)	0.0069 (6)	−0.0006 (6)
C7	0.0201 (7)	0.0191 (7)	0.0201 (7)	−0.0028 (6)	0.0054 (6)	−0.0004 (5)
C8	0.0192 (7)	0.0175 (7)	0.0211 (7)	−0.0023 (6)	0.0044 (6)	0.0028 (5)
C9	0.0198 (7)	0.0160 (7)	0.0197 (7)	−0.0020 (5)	0.0069 (6)	0.0004 (5)
C10	0.0175 (7)	0.0170 (7)	0.0212 (7)	0.0014 (5)	0.0054 (6)	0.0021 (5)
C11	0.0222 (7)	0.0195 (7)	0.0192 (7)	−0.0006 (6)	0.0059 (6)	0.0013 (6)

C12	0.0242 (8)	0.0227 (8)	0.0236 (8)	0.0035 (6)	0.0088 (6)	−0.0016 (6)
C13	0.0216 (7)	0.0199 (8)	0.0259 (8)	0.0026 (6)	0.0061 (6)	0.0019 (6)
C14	0.0394 (10)	0.0229 (9)	0.0378 (10)	0.0001 (7)	0.0165 (8)	−0.0068 (7)
C15	0.0205 (8)	0.0433 (11)	0.0336 (9)	0.0019 (7)	0.0092 (7)	0.0000 (8)
C16	0.0330 (9)	0.0381 (10)	0.0211 (8)	0.0055 (8)	0.0086 (7)	−0.0035 (7)

Geometric parameters (Å, º)

O1—C6	1.228 (2)	C5—C6	1.512 (2)
O2—C9	1.3733 (19)	C7—C8	1.463 (2)
O2—C14	1.433 (2)	C7—H7A	0.9300
O3—C10	1.3765 (18)	C8—C13	1.395 (2)
O3—C15	1.438 (2)	C8—C9	1.409 (2)
O4—C11	1.3634 (19)	C9—C10	1.397 (2)
O4—C16	1.436 (2)	C10—C11	1.409 (2)
N1—C3	1.335 (2)	C11—C12	1.397 (2)
N1—C2	1.346 (2)	C12—C13	1.387 (2)
N2—C6	1.345 (2)	C12—H12A	0.9300
N2—N3	1.3910 (18)	C13—H13A	0.9300
N2—H1N2	0.91 (3)	C14—H14A	0.9600
N3—C7	1.290 (2)	C14—H14B	0.9600
C1—C5	1.391 (2)	C14—H14C	0.9600
C1—C2	1.394 (2)	C15—H15A	0.9600
C1—H1A	0.9300	C15—H15B	0.9600
C2—H2A	0.9300	C15—H15C	0.9600
C3—C4	1.391 (2)	C16—H16A	0.9600
C3—H3A	0.9300	C16—H16B	0.9600
C4—C5	1.399 (2)	C16—H16C	0.9600
C4—H4A	0.9300		

C9—O2—C14	115.72 (13)	O2—C9—C8	118.64 (14)
C10—O3—C15	112.99 (13)	C10—C9—C8	120.32 (14)
C11—O4—C16	117.16 (13)	O3—C10—C9	120.87 (14)
C3—N1—C2	116.26 (15)	O3—C10—C11	119.46 (13)
C6—N2—N3	119.77 (13)	C9—C10—C11	119.68 (14)
C6—N2—H1N2	124.0 (15)	O4—C11—C12	124.39 (15)
N3—N2—H1N2	115.3 (15)	O4—C11—C10	115.49 (14)
C7—N3—N2	112.81 (13)	C12—C11—C10	120.11 (15)
C5—C1—C2	119.00 (16)	C13—C12—C11	119.48 (15)
C5—C1—H1A	120.5	C13—C12—H12A	120.3
C2—C1—H1A	120.5	C11—C12—H12A	120.3
N1—C2—C1	123.62 (16)	C12—C13—C8	121.61 (15)
N1—C2—H2A	118.2	C12—C13—H13A	119.2
C1—C2—H2A	118.2	C8—C13—H13A	119.2
N1—C3—C4	124.95 (16)	O2—C14—H14A	109.5
N1—C3—H3A	117.5	O2—C14—H14B	109.5
C4—C3—H3A	117.5	H14A—C14—H14B	109.5
C3—C4—C5	117.92 (16)	O2—C14—H14C	109.5

C3—C4—H4A	121.0	H14A—C14—H14C	109.5
C5—C4—H4A	121.0	H14B—C14—H14C	109.5
C1—C5—C4	118.23 (15)	O3—C15—H15A	109.5
C1—C5—C6	117.70 (15)	O3—C15—H15B	109.5
C4—C5—C6	124.06 (15)	H15A—C15—H15B	109.5
O1—C6—N2	123.99 (15)	O3—C15—H15C	109.5
O1—C6—C5	121.16 (14)	H15A—C15—H15C	109.5
N2—C6—C5	114.79 (14)	H15B—C15—H15C	109.5
N3—C7—C8	119.94 (14)	O4—C16—H16A	109.5
N3—C7—H7A	120.0	O4—C16—H16B	109.5
C8—C7—H7A	120.0	H16A—C16—H16B	109.5
C13—C8—C9	118.77 (14)	O4—C16—H16C	109.5
C13—C8—C7	121.20 (14)	H16A—C16—H16C	109.5
C9—C8—C7	119.90 (14)	H16B—C16—H16C	109.5
O2—C9—C10	120.87 (13)		

C6—N2—N3—C7	−165.58 (14)	C7—C8—C9—O2	7.4 (2)
C3—N1—C2—C1	0.3 (3)	C13—C8—C9—C10	−1.2 (2)
C5—C1—C2—N1	0.5 (3)	C7—C8—C9—C10	−177.24 (14)
C2—N1—C3—C4	−1.0 (3)	C15—O3—C10—C9	82.69 (18)
N1—C3—C4—C5	1.0 (3)	C15—O3—C10—C11	−97.83 (17)
C2—C1—C5—C4	−0.5 (2)	O2—C9—C10—O3	−5.1 (2)
C2—C1—C5—C6	−179.50 (14)	C8—C9—C10—O3	179.63 (14)
C3—C4—C5—C1	−0.2 (2)	O2—C9—C10—C11	175.45 (14)
C3—C4—C5—C6	178.75 (15)	C8—C9—C10—C11	0.2 (2)
N3—N2—C6—O1	7.8 (2)	C16—O4—C11—C12	−3.8 (2)
N3—N2—C6—C5	−175.09 (13)	C16—O4—C11—C10	176.28 (14)
C1—C5—C6—O1	27.6 (2)	O3—C10—C11—O4	1.7 (2)
C4—C5—C6—O1	−151.38 (17)	C9—C10—C11—O4	−178.79 (13)
C1—C5—C6—N2	−149.60 (15)	O3—C10—C11—C12	−178.17 (14)
C4—C5—C6—N2	31.5 (2)	C9—C10—C11—C12	1.3 (2)
N2—N3—C7—C8	−172.80 (13)	O4—C11—C12—C13	178.42 (15)
N3—C7—C8—C13	22.4 (2)	C10—C11—C12—C13	−1.7 (2)
N3—C7—C8—C9	−161.70 (15)	C11—C12—C13—C8	0.6 (2)
C14—O2—C9—C10	73.23 (19)	C9—C8—C13—C12	0.8 (2)
C14—O2—C9—C8	−111.40 (16)	C7—C8—C13—C12	176.81 (15)
C13—C8—C9—O2	−176.62 (14)		

Hydrogen-bond geometry (Å, º)

Cg1 is centroid of the C1/C2/N1/C3/C4/C5 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1*N*2···O1^{i}	0.91 (3)	2.09 (3)	2.7987 (19)	134 (2)
C4—H4*A*···O1^{i}	0.93	2.46	3.348 (2)	159
C14—H14*C*···O3	0.96	2.55	3.113 (2)	118
C15—H15*C*···O2^{ii}	0.96	2.49	3.292 (2)	141

C16—H16*A*···O3^{iii}	0.96	2.57	3.518 (2)	167
C14—H14*B*···*Cg*1^{i}	0.96	2.81	3.719 (3)	159

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