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N,1-Bis(4-ethoxyphenyl)-2,6-dimethyl-4-oxo-1,4-dihydropyridine-3-carboxamide

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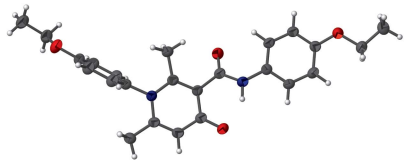
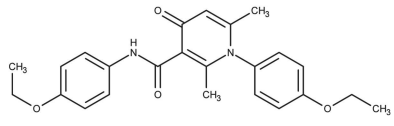
Structural data: full structural data are available from iucrdata.iucr.org

Condensation of ethyl acetoacetate and phenetidine gives the title compound, $C_{24}H_{26}N_2O_4$. The planar ethoxyphenyl group attached to the pyridine ring is twisted about 77.96 (11)° out of the plane of the *N*-ethoxycarboxamidopyridine unit. The carboxamide unit forms a dihedral angle of about 28.1 (2)° with the pyridine ring.

3D view



Chemical scheme



Structure description

Two molecules of the title compound (Fig. 1) fill the triclinic unit cell. The compound is composed of three planar rings with an intramolecular hydrogen bridge N21—H21···O17 (Table 1). The amide group is essentially planar [torsion angle O20—C19—N21—C22: 0.6 (3)°] but is twisted [O20—C19—C5—C6: −26.9 (3)°; C19—N21—C22—C27: 27.8 (3)°] out of the plane of the nearly coplanar pyridine and phenyl rings [dihedral angle between the mean planes of the pyridine and phenyl rings: 2.77 (10)°]. On the other hand, the *N*-phenyl pyridone linkage shows a large torsion angle [C12—C7—N1—C6: 76.0 (3)°]. Both ethoxy groups are nearly coplanar with the phenyl rings to which they are attached: the angle between the mean planes of the ethoxy groups and the aromatic ring on the amide side is 6.0 (2)° and on the pyridine side only 5.2 (2)°.

Synthesis and crystallization

The title compound was isolated as a side product in the formation of *p*-ethoxy acetoacetanilide, an intermediate in the 4-hydroxyquinoline synthesis according to Konrad–Limpach (Eicher & Hauptmann, 1994). A mixture of ethyl acetoacetate (40 ml) was heated in an open flask to 433 K and phenetidine (10 ml) was added slowly. After complete addition of the amine, strirring and heating was continued for 3 h. After cooling to ambient temperature, about 5 ml of diluted hydrochloric acid was added and the

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

D—H···A	D—H	H···A	D···A	D—H···A
N21—H21···O17	0.93 (2)	1.84 (2)	2.636 (2)	142.3 (18)

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{26}N_2O_4$
M_r	406.47
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	193
a, b, c (Å)	8.5516 (5), 11.5937 (7), 11.6637 (8)
α, β, γ (°)	64.268 (4), 79.206 (5), 84.288 (5)
V (Å^3)	1023.07 (12)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.73
Crystal size (mm)	0.17 × 0.11 × 0.04
Data collection	
Diffractometer	Stoe IPDS 2T
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10018, 3512, 2627
R_{int}	0.020
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.599
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.133, 1.07
No. of reflections	3512
No. of parameters	280
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.22

Computer programs: *X-RED* and *X-AREA* (Stoe & Cie, 1996), *SIR2004* (Altomare *et al.*, 1999), *SHELXL2018* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

mixture heated for further 3 h. After standing at 255 K for two weeks,the product crystallized as off-white crystals, m.p. = 484 K.

H-NMR (300 MHz; $CDCl_3$): δ**H** = δ [ppm] = 12.57 (*s*, 1H, N—H), 7.63–7.57 (*m*, 2H, Ph-2,6-H), 7.10–6.99 (*m*, 4H, Ph-2,3,5,6-H), 6.88–6.83 (*m*, 2H, Ph-3,5-H), 6.49 (*d*, 1H, ^4J = 0.88 Hz, 3-H py), 4.09 (*q*, 2H, ^3J = 6.98 Hz, O—CH_2–), 4.01 (*q*, 2H, ^3J = 6.96 Hz, O—CH_2), 2.53 (*s*, 3H, CH_3, 18-H), 1.93 (*d*, 3H, ^4J = 0.81 Hz, CH_3, 16-H), 1.47 (*t*, 3H, ^3J = 6.97 Hz, OEt-CH_3), 1.39 (*t*, 3H, ^3J = 6.97 Hz, OEt-CH_3); C-NMR (100 MHz; $CDCl_3$) δ**C** (75 MHz, $CDCl_3$): δ [ppm] = 178.11, 164.12, 159.81, 156.85, 155.36, 149.03, 132.31, 132.16, 128.83 (2 C, Ph), 122.34 (2 C, Ph), 119.01, 118.89 (=CH–), 115.95 (2 C, Ph), 114.73 (2 C, Ph), 64.14 (O—CH_2–), 63.77 (O—CH_2–), 21.93 (CH_3, C-16), 20.93 (CH_3, C-18), 15.03 (OEt—CH_3), 14.85 (OEt—CH_3). HR–ESI:[$C_{24}H_{26}N_2O_4$ + H]$^+$: calculated: 407.1966; found: 407.1962: IR: 3053, 2982, 2360, 2341, 1665, 1507, 1394, 1265, 1242, 1116, 1042, 825, 733, 703, 568 cm^{-1}.

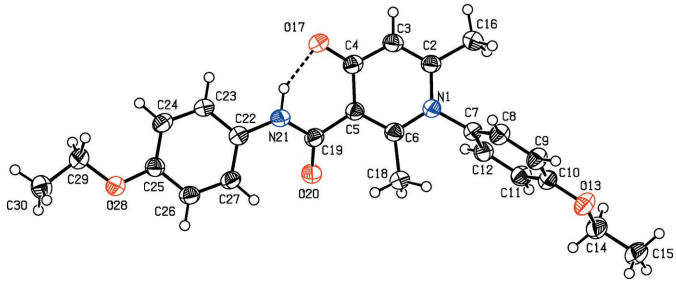

Figure 1
Perspective view of the title compound. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular hydrogen bond is drawn with a dashed line.

Refinement

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

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full crystallographic data

IUCrData (2018). **3**, x181640 [https://doi.org/10.1107/S2414314618016401]

N,1-Bis(4-ethoxyphenyl)-2,6-dimethyl-4-oxo-1,4-dihydropyridine-3-carboxamide

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Crystal data

$C_{24}H_{26}N_2O_4$
M_r = 406.47
Triclinic, $P\overline{1}$
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c = 11.6637 (8) Å
α = 64.268 (4)°
β = 79.206 (5)°
γ = 84.288 (5)°
V = 1023.07 (12) Å^3
Z = 2
$F(000)$ = 432
D_x = 1.319 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 15045 reflections
θ = 4.2–68.5°
μ = 0.73 mm^{-1}
T = 193 K
Column, colourless
0.17 × 0.11 × 0.04 mm

Data collection

Stoe IPDS 2T diffractometer
Radiation source: Incoatec microSource Cu
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
10018 measured reflections
3512 independent reflections
2627 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 67.4°, θ_{min} = 4.2°
h = −10→10
k = −13→13
l = −13→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.133
S = 1.07
3512 reflections
280 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 0.4717P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0077 (8)

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. Hydrogen atoms attached to carbons were placed at calculated positions and were refined in the riding-model approximation with isotropic displacement parameters set to 1.2 U_{eq}(C) or 1.5 U_{eq}(C_{methyl}). The hydrogen atom attached to N21 was localized in difference fourier maps and freely refined.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.6114 (2)	0.24526 (15)	0.58878 (15)	0.0341 (4)
C2	0.6827 (2)	0.35960 (18)	0.50480 (19)	0.0356 (5)
C3	0.6196 (2)	0.43617 (19)	0.3985 (2)	0.0378 (5)
H3	0.670348	0.514570	0.341388	0.045*
C4	0.4809 (2)	0.40539 (19)	0.36765 (19)	0.0361 (5)
C5	0.4176 (2)	0.27997 (18)	0.45280 (19)	0.0335 (5)
C6	0.4808 (2)	0.20510 (19)	0.56345 (19)	0.0358 (5)
C7	0.6766 (2)	0.16369 (19)	0.70529 (19)	0.0348 (5)
C8	0.6408 (3)	0.1903 (2)	0.8123 (2)	0.0398 (5)
H8	0.580126	0.264802	0.808302	0.048*
C9	0.6944 (3)	0.1071 (2)	0.9247 (2)	0.0419 (5)
H9	0.670703	0.124694	0.998513	0.050*
C10	0.7829 (3)	−0.00222 (19)	0.9311 (2)	0.0378 (5)
C11	0.8215 (3)	−0.0266 (2)	0.8232 (2)	0.0400 (5)
H11	0.884886	−0.099712	0.826294	0.048*
C12	0.7667 (3)	0.05662 (19)	0.7103 (2)	0.0374 (5)
H12	0.791426	0.039818	0.636068	0.045*
O13	0.8246 (2)	−0.07885 (14)	1.04879 (14)	0.0477 (4)
C14	0.9102 (3)	−0.1947 (2)	1.0638 (2)	0.0496 (6)
H14A	1.015694	−0.176305	1.008020	0.059*
H14B	0.850697	−0.247989	1.040183	0.059*
C15	0.9292 (3)	−0.2628 (2)	1.2037 (2)	0.0594 (7)
H15A	0.985524	−0.207879	1.226178	0.089*
H15B	0.990547	−0.342686	1.218401	0.089*
H15C	0.824002	−0.282321	1.257452	0.089*
C16	0.8280 (3)	0.3941 (2)	0.5366 (2)	0.0435 (5)
H16A	0.869917	0.474611	0.466589	0.065*
H16B	0.909150	0.325945	0.546832	0.065*
H16C	0.800155	0.404506	0.617015	0.065*
O17	0.42020 (18)	0.48431 (13)	0.27114 (14)	0.0426 (4)
C18	0.4110 (3)	0.0813 (2)	0.6649 (2)	0.0464 (6)
H18A	0.419455	0.074301	0.750386	0.070*
H18B	0.469156	0.009603	0.652010	0.070*
H18C	0.298650	0.079179	0.658792	0.070*
C19	0.2854 (3)	0.22908 (19)	0.42149 (19)	0.0365 (5)
O20	0.26641 (19)	0.11429 (13)	0.45822 (15)	0.0474 (4)

N21	0.1883 (2)	0.32054 (16)	0.34782 (17)	0.0366 (4)
H21	0.232 (3)	0.401 (2)	0.308 (2)	0.036 (6)*
C22	0.0552 (2)	0.29886 (19)	0.30477 (19)	0.0339 (5)
C23	0.0072 (2)	0.39391 (19)	0.19478 (19)	0.0384 (5)
H23	0.067046	0.469869	0.148539	0.046*
C24	−0.1265 (3)	0.3808 (2)	0.1505 (2)	0.0403 (5)
H24	−0.158216	0.447781	0.075200	0.048*
C25	−0.2137 (2)	0.26991 (19)	0.2161 (2)	0.0371 (5)
C26	−0.1668 (2)	0.17523 (19)	0.3272 (2)	0.0380 (5)
H26	−0.227335	0.099665	0.374036	0.046*
C27	−0.0346 (2)	0.18856 (19)	0.3710 (2)	0.0371 (5)
H27	−0.004113	0.122027	0.447092	0.044*
O28	−0.34753 (18)	0.24578 (14)	0.18180 (15)	0.0459 (4)
C29	−0.4047 (3)	0.3416 (2)	0.0713 (2)	0.0445 (6)
H29A	−0.327421	0.353552	−0.007505	0.053*
H29B	−0.419571	0.424171	0.078337	0.053*
C30	−0.5609 (3)	0.2979 (2)	0.0643 (2)	0.0477 (6)
H30A	−0.596022	0.355939	−0.017299	0.071*
H30B	−0.640747	0.298195	0.136424	0.071*
H30C	−0.547805	0.210922	0.069383	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0388 (9)	0.0323 (9)	0.0310 (9)	−0.0029 (7)	−0.0072 (7)	−0.0122 (7)
C2	0.0415 (11)	0.0308 (10)	0.0336 (11)	−0.0052 (8)	−0.0036 (9)	−0.0129 (9)
C3	0.0413 (12)	0.0326 (10)	0.0381 (11)	−0.0049 (9)	−0.0041 (9)	−0.0139 (9)
C4	0.0421 (12)	0.0320 (10)	0.0331 (11)	−0.0007 (9)	−0.0048 (9)	−0.0132 (9)
C5	0.0375 (11)	0.0300 (10)	0.0331 (11)	−0.0009 (8)	−0.0067 (9)	−0.0131 (9)
C6	0.0412 (12)	0.0327 (10)	0.0336 (11)	−0.0032 (9)	−0.0053 (9)	−0.0141 (9)
C7	0.0395 (11)	0.0318 (10)	0.0317 (11)	−0.0030 (8)	−0.0082 (9)	−0.0107 (9)
C8	0.0452 (12)	0.0383 (11)	0.0358 (11)	0.0037 (9)	−0.0070 (9)	−0.0166 (9)
C9	0.0517 (13)	0.0414 (12)	0.0350 (11)	0.0048 (10)	−0.0082 (10)	−0.0191 (10)
C10	0.0432 (12)	0.0356 (11)	0.0330 (11)	−0.0012 (9)	−0.0092 (9)	−0.0118 (9)
C11	0.0453 (12)	0.0360 (11)	0.0394 (12)	0.0003 (9)	−0.0067 (10)	−0.0171 (10)
C12	0.0435 (12)	0.0371 (11)	0.0341 (11)	−0.0019 (9)	−0.0057 (9)	−0.0175 (9)
O13	0.0617 (10)	0.0406 (8)	0.0379 (8)	0.0087 (7)	−0.0162 (7)	−0.0126 (7)
C14	0.0609 (15)	0.0351 (11)	0.0542 (14)	0.0060 (10)	−0.0234 (12)	−0.0162 (11)
C15	0.0764 (18)	0.0391 (13)	0.0550 (15)	0.0018 (12)	−0.0259 (14)	−0.0074 (11)
C16	0.0447 (13)	0.0418 (12)	0.0429 (12)	−0.0083 (10)	−0.0071 (10)	−0.0152 (10)
O17	0.0490 (9)	0.0327 (8)	0.0392 (8)	−0.0026 (6)	−0.0129 (7)	−0.0064 (7)
C18	0.0524 (14)	0.0405 (12)	0.0383 (12)	−0.0118 (10)	−0.0124 (10)	−0.0052 (10)
C19	0.0430 (12)	0.0315 (10)	0.0337 (11)	−0.0009 (9)	−0.0074 (9)	−0.0121 (9)
O20	0.0582 (10)	0.0300 (8)	0.0545 (10)	−0.0028 (7)	−0.0234 (8)	−0.0124 (7)
N21	0.0394 (10)	0.0276 (9)	0.0393 (10)	−0.0016 (7)	−0.0087 (8)	−0.0099 (8)
C22	0.0339 (11)	0.0332 (10)	0.0341 (11)	0.0016 (8)	−0.0041 (9)	−0.0148 (9)
C23	0.0416 (12)	0.0334 (11)	0.0341 (11)	−0.0063 (9)	−0.0049 (9)	−0.0083 (9)
C24	0.0462 (12)	0.0347 (11)	0.0341 (11)	0.0003 (9)	−0.0083 (9)	−0.0087 (9)

C25	0.0366 (11)	0.0351 (11)	0.0384 (11)	−0.0012 (9)	−0.0062 (9)	−0.0146 (9)
C26	0.0362 (11)	0.0315 (10)	0.0411 (12)	−0.0012 (8)	−0.0054 (9)	−0.0109 (9)
C27	0.0394 (11)	0.0294 (10)	0.0361 (11)	0.0005 (8)	−0.0064 (9)	−0.0083 (9)
O28	0.0437 (9)	0.0394 (8)	0.0479 (9)	−0.0048 (7)	−0.0162 (7)	−0.0082 (7)
C29	0.0497 (13)	0.0392 (11)	0.0421 (12)	0.0003 (10)	−0.0152 (10)	−0.0120 (10)
C30	0.0430 (13)	0.0515 (13)	0.0526 (14)	0.0028 (10)	−0.0117 (11)	−0.0251 (11)

Geometric parameters (Å, º)

N1—C6	1.378 (3)	C15—H15C	0.9800
N1—C2	1.378 (2)	C16—H16A	0.9800
N1—C7	1.455 (2)	C16—H16B	0.9800
C2—C3	1.348 (3)	C16—H16C	0.9800
C2—C16	1.497 (3)	C18—H18A	0.9800
C3—C4	1.421 (3)	C18—H18B	0.9800
C3—H3	0.9500	C18—H18C	0.9800
C4—O17	1.266 (2)	C19—O20	1.226 (2)
C4—C5	1.447 (3)	C19—N21	1.362 (3)
C5—C6	1.380 (3)	N21—C22	1.411 (3)
C5—C19	1.495 (3)	N21—H21	0.93 (2)
C6—C18	1.499 (3)	C22—C23	1.381 (3)
C7—C12	1.379 (3)	C22—C27	1.392 (3)
C7—C8	1.386 (3)	C23—C24	1.386 (3)
C8—C9	1.377 (3)	C23—H23	0.9500
C8—H8	0.9500	C24—C25	1.385 (3)
C9—C10	1.390 (3)	C24—H24	0.9500
C9—H9	0.9500	C25—O28	1.371 (3)
C10—O13	1.364 (2)	C25—C26	1.385 (3)
C10—C11	1.382 (3)	C26—C27	1.372 (3)
C11—C12	1.386 (3)	C26—H26	0.9500
C11—H11	0.9500	C27—H27	0.9500
C12—H12	0.9500	O28—C29	1.421 (2)
O13—C14	1.421 (3)	C29—C30	1.503 (3)
C14—C15	1.506 (3)	C29—H29A	0.9900
C14—H14A	0.9900	C29—H29B	0.9900
C14—H14B	0.9900	C30—H30A	0.9800
C15—H15A	0.9800	C30—H30B	0.9800
C15—H15B	0.9800	C30—H30C	0.9800
C6—N1—C2	121.30 (17)	C2—C16—H16A	109.5
C6—N1—C7	119.08 (16)	C2—C16—H16B	109.5
C2—N1—C7	119.62 (17)	H16A—C16—H16B	109.5
C3—C2—N1	119.37 (19)	C2—C16—H16C	109.5
C3—C2—C16	122.52 (18)	H16A—C16—H16C	109.5
N1—C2—C16	118.11 (18)	H16B—C16—H16C	109.5
C2—C3—C4	123.21 (19)	C6—C18—H18A	109.5
C2—C3—H3	118.4	C6—C18—H18B	109.5
C4—C3—H3	118.4	H18A—C18—H18B	109.5

O17—C4—C3	120.80 (19)	C6—C18—H18C	109.5
O17—C4—C5	123.77 (19)	H18A—C18—H18C	109.5
C3—C4—C5	115.44 (18)	H18B—C18—H18C	109.5
C6—C5—C4	120.07 (19)	O20—C19—N21	122.6 (2)
C6—C5—C19	119.21 (17)	O20—C19—C5	122.82 (18)
C4—C5—C19	120.72 (17)	N21—C19—C5	114.62 (17)
N1—C6—C5	120.25 (18)	C19—N21—C22	126.21 (18)
N1—C6—C18	115.91 (18)	C19—N21—H21	113.0 (13)
C5—C6—C18	123.79 (19)	C22—N21—H21	118.8 (13)
C12—C7—C8	120.58 (19)	C23—C22—C27	118.25 (19)
C12—C7—N1	119.52 (19)	C23—C22—N21	118.56 (18)
C8—C7—N1	119.81 (18)	C27—C22—N21	123.13 (18)
C9—C8—C7	119.1 (2)	C22—C23—C24	121.41 (19)
C9—C8—H8	120.5	C22—C23—H23	119.3
C7—C8—H8	120.5	C24—C23—H23	119.3
C8—C9—C10	120.7 (2)	C25—C24—C23	119.87 (19)
C8—C9—H9	119.7	C25—C24—H24	120.1
C10—C9—H9	119.7	C23—C24—H24	120.1
O13—C10—C11	124.96 (19)	O28—C25—C24	125.27 (19)
O13—C10—C9	115.05 (19)	O28—C25—C26	115.94 (18)
C11—C10—C9	120.00 (19)	C24—C25—C26	118.8 (2)
C10—C11—C12	119.3 (2)	C27—C26—C25	121.21 (19)
C10—C11—H11	120.3	C27—C26—H26	119.4
C12—C11—H11	120.3	C25—C26—H26	119.4
C7—C12—C11	120.3 (2)	C26—C27—C22	120.47 (19)
C7—C12—H12	119.8	C26—C27—H27	119.8
C11—C12—H12	119.8	C22—C27—H27	119.8
C10—O13—C14	118.15 (18)	C25—O28—C29	118.43 (16)
O13—C14—C15	106.4 (2)	O28—C29—C30	107.59 (18)
O13—C14—H14A	110.4	O28—C29—H29A	110.2
C15—C14—H14A	110.4	C30—C29—H29A	110.2
O13—C14—H14B	110.4	O28—C29—H29B	110.2
C15—C14—H14B	110.4	C30—C29—H29B	110.2
H14A—C14—H14B	108.6	H29A—C29—H29B	108.5
C14—C15—H15A	109.5	C29—C30—H30A	109.5
C14—C15—H15B	109.5	C29—C30—H30B	109.5
H15A—C15—H15B	109.5	H30A—C30—H30B	109.5
C14—C15—H15C	109.5	C29—C30—H30C	109.5
H15A—C15—H15C	109.5	H30A—C30—H30C	109.5
H15B—C15—H15C	109.5	H30B—C30—H30C	109.5

C6—N1—C2—C3	2.8 (3)	O13—C10—C11—C12	177.6 (2)
C7—N1—C2—C3	−178.49 (19)	C9—C10—C11—C12	−2.1 (3)
C6—N1—C2—C16	−177.64 (19)	C8—C7—C12—C11	0.6 (3)
C7—N1—C2—C16	1.1 (3)	N1—C7—C12—C11	−175.92 (19)
N1—C2—C3—C4	0.2 (3)	C10—C11—C12—C7	0.9 (3)
C16—C2—C3—C4	−179.4 (2)	C11—C10—O13—C14	−1.9 (3)
C2—C3—C4—O17	175.3 (2)	C9—C10—O13—C14	177.8 (2)

C2—C3—C4—C5	−5.0 (3)	C10—O13—C14—C15	−176.1 (2)
O17—C4—C5—C6	−173.2 (2)	C6—C5—C19—O20	−26.9 (3)
C3—C4—C5—C6	7.1 (3)	C4—C5—C19—O20	152.3 (2)
O17—C4—C5—C19	7.7 (3)	C6—C5—C19—N21	153.68 (19)
C3—C4—C5—C19	−171.97 (19)	C4—C5—C19—N21	−27.2 (3)
C2—N1—C6—C5	−0.5 (3)	O20—C19—N21—C22	0.6 (3)
C7—N1—C6—C5	−179.22 (18)	C5—C19—N21—C22	−179.97 (18)
C2—N1—C6—C18	−177.83 (19)	C19—N21—C22—C23	−155.2 (2)
C7—N1—C6—C18	3.5 (3)	C19—N21—C22—C27	27.8 (3)
C4—C5—C6—N1	−4.6 (3)	C27—C22—C23—C24	−0.1 (3)
C19—C5—C6—N1	174.49 (18)	N21—C22—C23—C24	−177.27 (19)
C4—C5—C6—C18	172.5 (2)	C22—C23—C24—C25	−0.8 (3)
C19—C5—C6—C18	−8.4 (3)	C23—C24—C25—O28	−180.0 (2)
C6—N1—C7—C12	76.0 (3)	C23—C24—C25—C26	1.6 (3)
C2—N1—C7—C12	−102.7 (2)	O28—C25—C26—C27	179.93 (19)
C6—N1—C7—C8	−100.6 (2)	C24—C25—C26—C27	−1.5 (3)
C2—N1—C7—C8	80.7 (2)	C25—C26—C27—C22	0.6 (3)
C12—C7—C8—C9	−1.0 (3)	C23—C22—C27—C26	0.2 (3)
N1—C7—C8—C9	175.53 (19)	N21—C22—C27—C26	177.24 (19)
C7—C8—C9—C10	−0.2 (3)	C24—C25—O28—C29	−0.8 (3)
C8—C9—C10—O13	−178.0 (2)	C26—C25—O28—C29	177.67 (19)
C8—C9—C10—C11	1.7 (3)	C25—O28—C29—C30	−173.54 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21—H21···O17	0.93 (2)	1.84 (2)	2.636 (2)	142.3 (18)