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(*E*)-*N*-{3-[(*m*-Tolylimino)methyl]pyridin-2-yl}-pivalamide

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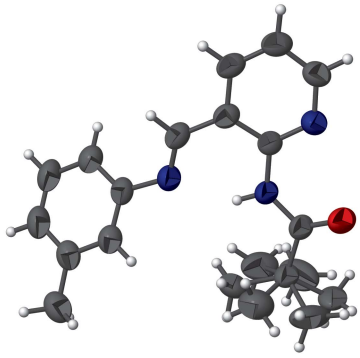
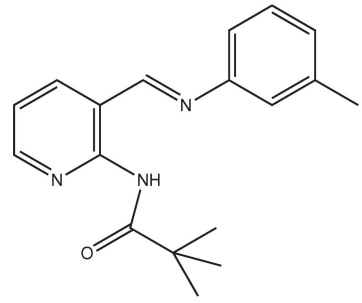
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{18}H_{21}N_3O$, the dihedral angle between the pyridine and benzene rings is 30.53 (7)° and the C—C=N—C torsion angle is −170.6 (2)°. An intramolecular N—H···N hydrogen bond generates an *S*(6) ring. In the crystal, very weak C—H···O hydrogen bonds link the molecules into *C*(8) [101] chains. The *tert*-butyl methyl groups are disordered over two sets of sites in a 0.783 (4):0.217 (4) ratio.

3D view



Chemical scheme



Structure description

Schiff bases were first reported by Hugo Schiff in 1864. As part of our studies in this area, we herein report the synthesis and structure of the title compound (Fig. 1).

The dihedral angle between the pyridine (N2/C9–C13) and benzene (C2–C7) ring systems is 30.53 (7)°. The molecular structure features an intramolecular N—H···N hydrogen bond, which generates an *S*(6) ring. The C—N bond distances of the imino-group atoms [C6—N1 = 1.420 (3) Å and C8═N1 = 1.273 (3) Å] are consistent with those in related structures such as 2,4-dichloro-*N*-[(*E*)-(5-nitrothiophen-2-yl) methylidene]aniline (Köysal *et al.*, 2016).

In the crystal, weak C11—H11···O1 hydrogen bonds (Table 1, Fig. 2) link the molecules into [101] chains.

Synthesis and crystallization

Solutions of *N*-(5-formylpyridin-2-yl)pivalamide (0.020 g, 0.96 mmol) in 20 ml ethanol and *o*-toluidine (0.0107 g, 0.90 mmol) in 20 ml ethanol were mixed and stirred for 1 h under reflux. Colourless needles were recovered upon slow evaporation of the solvent (yield 60%; m.p 457–459 K).

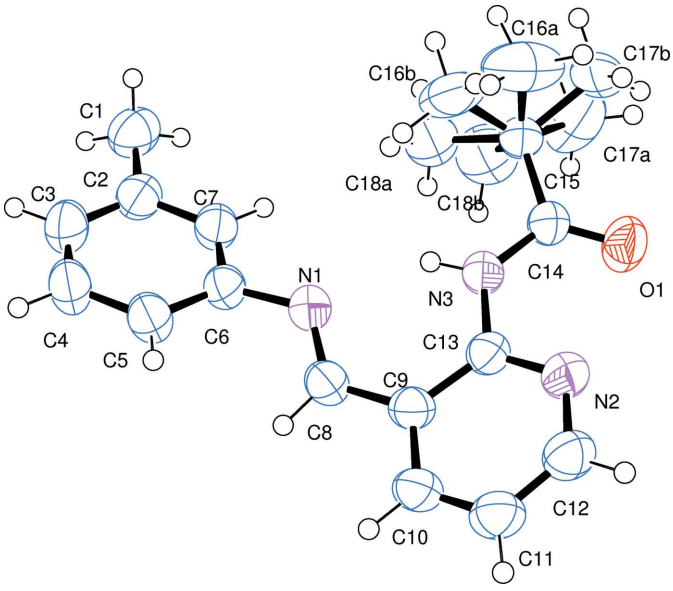


Figure 1
The molecular structure, showing 50% probability displacement ellipsoids. Both orientations of the disordered *tert*-butyl group are shown.

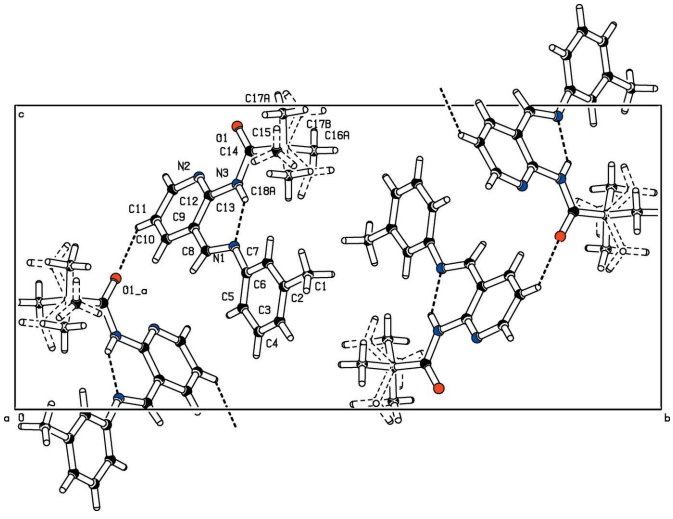


Figure 2
The packing, viewed down [100], showing the hydrogen-bonding interactions (dashed lines).

Refinement

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

Acknowledgements

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···N1	0.86 (3)	2.00 (3)	2.744 (3)	145 (3)
C11—H11···O1^{i}	0.93	2.61	3.404 (4)	144

Symmetry code: (i) $x-1, -y+\frac{1}{2}, z-\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{21}N_3O$
M_r	295.38
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	5.572 (3), 24.9671 (11), 12.2380 (5)
β (°)	106.529 (3)
V (Å^3)	1632.1 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.51 × 0.21 × 0.01
Data collection	
Diffractometer	STOE IPDS 2
Absorption correction	Integration *X-RED32* (Stoe & Cie, 2002)
T_{min}, T_{max}	0.969, 0.993
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19913, 2957, 1820
R_{int}	0.088
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.600
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.151, 1.02
No. of reflections	2957
No. of parameters	237
No. of restraints	127
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.24

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2002), *SHELXT2016/6* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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full crystallographic data

IUCrData (2017). **2**, x171702 [https://doi.org/10.1107/S2414314617017023]

(*E*)-*N*-{3-[(*m*-Tolylimino)methyl]pyridin-2-yl}pivalamide

Şehriman Atalay, Semra Gerçeker and Seher Meral

(*E*)-*N*-{3-[(*m*-Tolylimino)methyl]pyridin-2-yl}pivalamide

Crystal data

$C_{18}H_{21}N_3O$
M_r = 295.38
Monoclinic, $P2_1/c$
a = 5.572 (3) Å
b = 24.9671 (11) Å
c = 12.2380 (5) Å
β = 106.529 (3)°
V = 1632.1 (7) Å^3
Z = 4
$F(000)$ = 632
D_x = 1.202 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 16183 reflections
θ = 1.6–26.5°
μ = 0.08 mm^{-1}
T = 293 K
Needle, colorless
0.51 × 0.21 × 0.01 mm

Data collection

STOE IPDS 2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Detector resolution: 6.67 pixels mm^{-1}
w scans
Absorption correction: integration X-RED32 (Stoe & Cie, 2002)
T_{min} = 0.969, T_{max} = 0.993
19913 measured reflections
2957 independent reflections
1820 reflections with $I > 2\sigma(I)$
R_{int} = 0.088
θ_{max} = 25.3°, θ_{min} = 1.6°
h = −6→6
k = −29→29
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.151
S = 1.02
2957 reflections
237 parameters
127 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0694P)^2 + 0.1577P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 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. The H3 and H11 atoms bonded to N3 and C11 were freely refined. All other H atoms were positioned geometrically and rifined using a riding model, with C—H distances of 0.93 Å and methyl C—H distances 0.96 Å.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.0148 (4)	0.34395 (8)	0.93073 (15)	0.0765 (7)	
N1	0.0847 (4)	0.33938 (9)	0.53592 (17)	0.0543 (6)	
N2	−0.3301 (4)	0.28489 (9)	0.76396 (18)	0.0582 (6)	
N3	−0.0212 (5)	0.34425 (9)	0.74136 (19)	0.0563 (6)	
C1	0.7176 (6)	0.45364 (12)	0.4428 (3)	0.0762 (9)	
H1A	0.661209	0.489716	0.447020	0.114*	
H1B	0.814125	0.451961	0.389229	0.114*	
H1C	0.819411	0.442612	0.516564	0.114*	
C2	0.4947 (5)	0.41701 (11)	0.4044 (2)	0.0596 (7)	
C3	0.3744 (7)	0.40961 (13)	0.2903 (3)	0.0732 (9)	
H3A	0.436555	0.426282	0.235999	0.088*	
C4	0.1643 (7)	0.37802 (13)	0.2552 (2)	0.0734 (9)	
H4A	0.086189	0.373619	0.177745	0.088*	
C5	0.0679 (6)	0.35273 (11)	0.3341 (2)	0.0625 (7)	
H5	−0.074962	0.331639	0.309921	0.075*	
C6	0.1859 (5)	0.35905 (10)	0.4495 (2)	0.0533 (7)	
C7	0.3986 (5)	0.39123 (11)	0.4825 (2)	0.0572 (7)	
H7	0.478515	0.395498	0.559810	0.069*	
C8	−0.0425 (5)	0.29625 (11)	0.5208 (2)	0.0560 (7)	
H8	−0.045267	0.275629	0.457161	0.067*	
C9	−0.1845 (5)	0.27694 (10)	0.5967 (2)	0.0516 (6)	
C10	−0.3483 (6)	0.23469 (11)	0.5595 (2)	0.0612 (8)	
H10	−0.354012	0.217390	0.491512	0.073*	
C11	−0.5023 (6)	0.21830 (12)	0.6229 (2)	0.0659 (8)	
H11	−0.614229	0.190184	0.598442	0.079*	
C12	−0.4870 (5)	0.24440 (11)	0.7229 (2)	0.0631 (8)	
H12	−0.592703	0.233252	0.765170	0.076*	
C13	−0.1813 (5)	0.30095 (9)	0.7022 (2)	0.0491 (6)	
C14	0.0607 (5)	0.36424 (10)	0.8489 (2)	0.0525 (6)	
C15	0.2151 (5)	0.41602 (10)	0.8613 (2)	0.0571 (7)	
C16A	0.0395 (9)	0.46332 (15)	0.8459 (7)	0.1140 (19)	0.783 (4)
H16A	0.129858	0.495653	0.841931	0.171*	0.783 (4)
H16B	−0.029205	0.465312	0.909403	0.171*	0.783 (4)
H16C	−0.093634	0.459038	0.776741	0.171*	0.783 (4)
C17A	0.4209 (10)	0.4148 (2)	0.9742 (4)	0.115 (2)	0.783 (4)
H17A	0.522650	0.383497	0.977020	0.172*	0.783 (4)
H17B	0.346685	0.413798	1.036013	0.172*	0.783 (4)
H17C	0.522916	0.446261	0.980700	0.172*	0.783 (4)
C18A	0.3581 (8)	0.42136 (18)	0.7721 (4)	0.0810 (13)	0.783 (4)
H18A	0.464112	0.452371	0.788654	0.122*	0.783 (4)
H18B	0.241203	0.425071	0.697804	0.122*	0.783 (4)
H18C	0.458626	0.389982	0.773700	0.122*	0.783 (4)
C16B	0.090 (3)	0.4532 (5)	0.7612 (13)	0.094 (4)	0.217 (4)
H16D	−0.077479	0.461039	0.762392	0.141*	0.217 (4)
H16E	0.184157	0.485869	0.767965	0.141*	0.217 (4)

H16F	0.086620	0.435823	0.690736	0.141*	0.217 (4)
C17B	0.171 (4)	0.4469 (5)	0.9637 (13)	0.088 (4)	0.217 (4)
H17D	0.227235	0.483230	0.962648	0.132*	0.217 (4)
H17E	0.263494	0.430012	1.033458	0.132*	0.217 (4)
H17F	−0.003913	0.446646	0.958390	0.132*	0.217 (4)
C18B	0.4808 (15)	0.4025 (5)	0.8628 (18)	0.101 (4)	0.217 (4)
H18D	0.488336	0.365988	0.839495	0.151*	0.217 (4)
H18E	0.589883	0.407175	0.938581	0.151*	0.217 (4)
H18F	0.532814	0.425795	0.811415	0.151*	0.217 (4)
H3	0.044 (5)	0.3550 (11)	0.690 (2)	0.062 (8)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0948 (16)	0.0850 (14)	0.0462 (11)	−0.0347 (12)	0.0143 (10)	0.0012 (10)
N1	0.0632 (15)	0.0538 (14)	0.0484 (12)	−0.0040 (12)	0.0196 (11)	−0.0008 (10)
N2	0.0647 (15)	0.0543 (13)	0.0571 (13)	−0.0130 (12)	0.0200 (11)	−0.0020 (10)
N3	0.0737 (16)	0.0524 (13)	0.0455 (12)	−0.0199 (12)	0.0214 (11)	−0.0067 (10)
C1	0.079 (2)	0.068 (2)	0.091 (2)	0.0003 (17)	0.0400 (18)	0.0070 (16)
C2	0.0664 (19)	0.0541 (16)	0.0658 (18)	0.0112 (14)	0.0309 (15)	0.0055 (13)
C3	0.095 (3)	0.073 (2)	0.0622 (19)	0.0041 (19)	0.0403 (18)	0.0064 (15)
C4	0.097 (2)	0.080 (2)	0.0483 (16)	0.007 (2)	0.0279 (16)	0.0018 (15)
C5	0.0720 (19)	0.0660 (17)	0.0506 (16)	0.0018 (15)	0.0191 (14)	−0.0040 (13)
C6	0.0647 (17)	0.0504 (15)	0.0492 (15)	0.0058 (14)	0.0233 (13)	0.0014 (12)
C7	0.0660 (18)	0.0557 (16)	0.0523 (15)	0.0079 (14)	0.0208 (14)	0.0042 (12)
C8	0.0698 (19)	0.0518 (16)	0.0450 (14)	0.0023 (14)	0.0142 (13)	−0.0038 (12)
C9	0.0598 (17)	0.0430 (14)	0.0482 (14)	0.0008 (12)	0.0095 (12)	−0.0009 (11)
C10	0.078 (2)	0.0486 (16)	0.0513 (15)	−0.0087 (14)	0.0096 (14)	−0.0065 (12)
C11	0.070 (2)	0.0563 (17)	0.0643 (18)	−0.0137 (15)	0.0085 (15)	−0.0027 (14)
C12	0.0618 (18)	0.0599 (17)	0.0679 (18)	−0.0120 (15)	0.0189 (15)	0.0008 (14)
C13	0.0560 (16)	0.0448 (14)	0.0447 (13)	−0.0033 (12)	0.0113 (12)	0.0027 (11)
C14	0.0636 (17)	0.0497 (14)	0.0432 (14)	−0.0042 (12)	0.0136 (12)	0.0010 (11)
C15	0.0727 (18)	0.0482 (14)	0.0516 (14)	−0.0143 (13)	0.0195 (13)	−0.0057 (11)
C16A	0.096 (3)	0.066 (3)	0.192 (6)	−0.004 (2)	0.059 (4)	−0.023 (3)
C17A	0.134 (4)	0.115 (4)	0.069 (3)	−0.072 (3)	−0.015 (3)	0.010 (3)
C18A	0.080 (3)	0.082 (3)	0.086 (3)	−0.035 (2)	0.032 (2)	−0.012 (2)
C16B	0.121 (8)	0.050 (6)	0.102 (7)	−0.023 (6)	0.015 (7)	0.004 (6)
C17B	0.121 (8)	0.066 (7)	0.090 (6)	−0.053 (7)	0.049 (6)	−0.034 (5)
C18B	0.088 (6)	0.106 (8)	0.107 (9)	−0.022 (6)	0.025 (6)	−0.012 (7)

Geometric parameters (Å, º)

O1—C14	1.213 (3)	C11—C12	1.368 (4)
N1—C8	1.273 (3)	C11—H11	0.9300
N1—C6	1.420 (3)	C12—H12	0.9300
N2—C13	1.333 (3)	C14—C15	1.536 (4)
N2—C12	1.338 (3)	C15—C16A	1.511 (4)
N3—C14	1.359 (3)	C15—C18B	1.513 (7)

N3—C13	1.397 (3)	C15—C17A	1.524 (4)
N3—H3	0.86 (3)	C15—C18A	1.530 (4)
C1—C2	1.506 (4)	C15—C16B	1.536 (7)
C1—H1A	0.9600	C15—C17B	1.549 (6)
C1—H1B	0.9600	C16A—H16A	0.9600
C1—H1C	0.9600	C16A—H16B	0.9600
C2—C3	1.380 (4)	C16A—H16C	0.9600
C2—C7	1.380 (4)	C17A—H17A	0.9600
C3—C4	1.375 (4)	C17A—H17B	0.9600
C3—H3A	0.9300	C17A—H17C	0.9600
C4—C5	1.384 (4)	C18A—H18A	0.9600
C4—H4A	0.9300	C18A—H18B	0.9600
C5—C6	1.387 (4)	C18A—H18C	0.9600
C5—H5	0.9300	C16B—H16D	0.9600
C6—C7	1.393 (4)	C16B—H16E	0.9600
C7—H7	0.9300	C16B—H16F	0.9600
C8—C9	1.462 (4)	C17B—H17D	0.9600
C8—H8	0.9300	C17B—H17E	0.9600
C9—C10	1.384 (4)	C17B—H17F	0.9600
C9—C13	1.419 (3)	C18B—H18D	0.9600
C10—C11	1.373 (4)	C18B—H18E	0.9600
C10—H10	0.9300	C18B—H18F	0.9600

C8—N1—C6	120.4 (2)	N3—C14—C15	115.4 (2)
C13—N2—C12	117.4 (2)	C16A—C15—C17A	115.0 (4)
C14—N3—C13	128.5 (2)	C16A—C15—C18A	107.1 (4)
C14—N3—H3	120.2 (19)	C17A—C15—C18A	103.8 (3)
C13—N3—H3	110.7 (18)	C18B—C15—C16B	111.3 (11)
C2—C1—H1A	109.5	C16A—C15—C14	108.7 (3)
C2—C1—H1B	109.5	C18B—C15—C14	109.4 (5)
H1A—C1—H1B	109.5	C17A—C15—C14	109.1 (2)
C2—C1—H1C	109.5	C18A—C15—C14	113.2 (2)
H1A—C1—H1C	109.5	C16B—C15—C14	108.4 (5)
H1B—C1—H1C	109.5	C18B—C15—C17B	118.7 (10)
C3—C2—C7	117.8 (3)	C16B—C15—C17B	101.8 (11)
C3—C2—C1	121.1 (3)	C14—C15—C17B	106.6 (4)
C7—C2—C1	121.0 (3)	C15—C16A—H16A	109.5
C4—C3—C2	121.2 (3)	C15—C16A—H16B	109.5
C4—C3—H3A	119.4	H16A—C16A—H16B	109.5
C2—C3—H3A	119.4	C15—C16A—H16C	109.5
C3—C4—C5	120.6 (3)	H16A—C16A—H16C	109.5
C3—C4—H4A	119.7	H16B—C16A—H16C	109.5
C5—C4—H4A	119.7	C15—C17A—H17A	109.5
C4—C5—C6	119.6 (3)	C15—C17A—H17B	109.5
C4—C5—H5	120.2	H17A—C17A—H17B	109.5
C6—C5—H5	120.2	C15—C17A—H17C	109.5
C5—C6—C7	118.6 (2)	H17A—C17A—H17C	109.5
C5—C6—N1	123.0 (3)	H17B—C17A—H17C	109.5

C7—C6—N1	118.0 (2)	C15—C18A—H18A	109.5
C2—C7—C6	122.3 (3)	C15—C18A—H18B	109.5
C2—C7—H7	118.9	H18A—C18A—H18B	109.5
C6—C7—H7	118.9	C15—C18A—H18C	109.5
N1—C8—C9	124.5 (2)	H18A—C18A—H18C	109.5
N1—C8—H8	117.8	H18B—C18A—H18C	109.5
C9—C8—H8	117.8	C15—C16B—H16D	109.5
C10—C9—C13	117.2 (2)	C15—C16B—H16E	109.5
C10—C9—C8	117.9 (2)	H16D—C16B—H16E	109.5
C13—C9—C8	124.7 (2)	C15—C16B—H16F	109.5
C11—C10—C9	120.1 (3)	H16D—C16B—H16F	109.5
C11—C10—H10	120.0	H16E—C16B—H16F	109.5
C9—C10—H10	120.0	C15—C17B—H17D	109.5
C12—C11—C10	118.3 (3)	C15—C17B—H17E	109.5
C12—C11—H11	120.9	H17D—C17B—H17E	109.5
C10—C11—H11	120.9	C15—C17B—H17F	109.5
N2—C12—C11	124.3 (3)	H17D—C17B—H17F	109.5
N2—C12—H12	117.8	H17E—C17B—H17F	109.5
C11—C12—H12	117.8	C15—C18B—H18D	109.5
N2—C13—N3	118.5 (2)	C15—C18B—H18E	109.5
N2—C13—C9	122.7 (2)	H18D—C18B—H18E	109.5
N3—C13—C9	118.7 (2)	C15—C18B—H18F	109.5
O1—C14—N3	123.7 (2)	H18D—C18B—H18F	109.5
O1—C14—C15	120.9 (2)	H18E—C18B—H18F	109.5

C7—C2—C3—C4	0.6 (4)	C12—N2—C13—C9	0.0 (4)
C1—C2—C3—C4	−177.1 (3)	C14—N3—C13—N2	20.5 (4)
C2—C3—C4—C5	0.0 (5)	C14—N3—C13—C9	−161.5 (3)
C3—C4—C5—C6	−0.5 (4)	C10—C9—C13—N2	−1.0 (4)
C4—C5—C6—C7	0.4 (4)	C8—C9—C13—N2	174.0 (2)
C4—C5—C6—N1	172.9 (3)	C10—C9—C13—N3	−179.0 (2)
C8—N1—C6—C5	33.4 (4)	C8—C9—C13—N3	−4.0 (4)
C8—N1—C6—C7	−154.0 (3)	C13—N3—C14—O1	4.9 (5)
C3—C2—C7—C6	−0.7 (4)	C13—N3—C14—C15	−174.0 (2)
C1—C2—C7—C6	177.0 (2)	O1—C14—C15—C16A	−88.8 (4)
C5—C6—C7—C2	0.2 (4)	N3—C14—C15—C16A	90.1 (4)
N1—C6—C7—C2	−172.7 (2)	O1—C14—C15—C18B	101.5 (9)
C6—N1—C8—C9	−170.6 (2)	N3—C14—C15—C18B	−79.6 (9)
N1—C8—C9—C10	168.9 (3)	O1—C14—C15—C17A	37.3 (4)
N1—C8—C9—C13	−6.0 (4)	N3—C14—C15—C17A	−143.8 (4)
C13—C9—C10—C11	1.2 (4)	O1—C14—C15—C18A	152.4 (3)
C8—C9—C10—C11	−174.1 (3)	N3—C14—C15—C18A	−28.7 (4)
C9—C10—C11—C12	−0.6 (4)	O1—C14—C15—C16B	−136.9 (10)
C13—N2—C12—C11	0.7 (4)	N3—C14—C15—C16B	42.0 (10)
C10—C11—C12—N2	−0.4 (4)	O1—C14—C15—C17B	−28.0 (10)
C12—N2—C13—N3	178.0 (2)	N3—C14—C15—C17B	150.9 (9)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···N1	0.86 (3)	2.00 (3)	2.744 (3)	145 (3)
C11—H11···O1^{i}	0.93	2.61	3.404 (4)	144

Symmetry code: (i) $x-1, -y+1/2, z-1/2$.