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N-(3-{[(*Z*)-(3-Hydroxy-4-methylphenyl)imino]methyl}pyridin-2-yl)pivalamide

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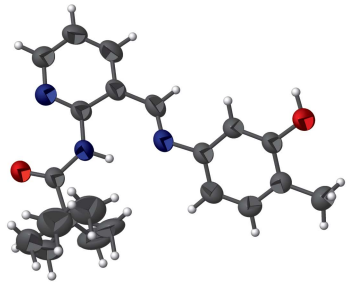
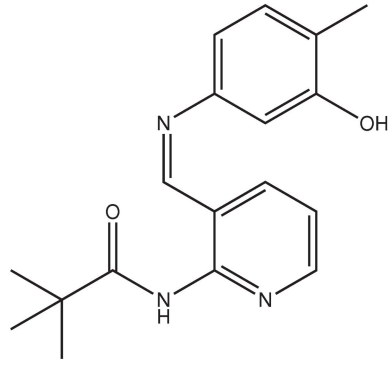
The molecular structure of the title compound, $C_{18}H_{21}N_3O_2$, contains pivalamide, pyridin and hydroxy-methylphenyl moieties. The whole molecule is not planar, the dihedral angle between the benzene rings being 34.84 (7)°. The molecular conformation is stabilized by an intramolecular N—H···N hydrogen bond. In the crystal, molecules are linked by O—H···O, O—H···N and C—H···O hydrogen bonds. The C and H atoms of the *tert*-butyl group disordered over two sets of sites with an occupancy ratio of 0.692 (5):0.308 (5).

3D view



Chemical scheme



Structure description

Schiff bases have wide applications according to their biological activities and chemical characteristics. They have been used as model systems for biological macromolecules and have shown anticancer, antioxic, anti-inflammatory and antibacterial properties (Chen & Rhodes, 1996; Uhlenbrock *et al.*, 1996; Anderson *et al.*, 1997; Singh, 1999; Ambike *et al.*, 2007). Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Hadjoudis *et al.*, 1987). We herein report the molecular structure of $C_{18}H_{21}N_3O_2$ (I), which shows Schiff base character.

The molecular structure (Fig. 1) is not planar, the dihedral angle between the C2–C7 and N2/C9–C13 rings being 34.84 (7)°. The maximum deviation from planarity in the latter ring is 0.097 (2) Å for atom C9. The bond lengths involving imino group atoms [N1—C5 = 1.421 (3) and N1—C8 = 1.272 (3) Å] are consistent with those in the related structures 2-[(2-bromophenyl)iminomethyl]-6-methylphenol (Karadağ *et al.*, 2010) and (*E*)-4-bromo-2-[(4-ethylphenyliminomethyl]phenol (Atalay *et al.*, 2008). An intramolecular N3—H3···N1 hydrogen bond (Table 1) closes an *R*(6) ring.

In the crystal, molecules are linked by O—H···O, C—H···O and O—H···N hydrogen bonds, with the same atom, O2, acting as the acceptor for the first two of these inter-

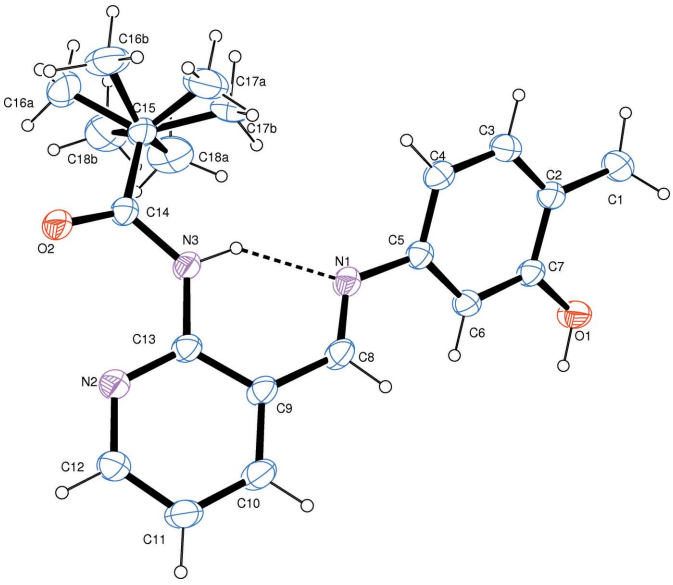


Figure 1
A view of the moieties of (I), with the atom-numbering scheme and 20% probability displacement ellipsoids. The intramolecular hydrogen bond is shown as a dashed line.

actions. The O1—H1···N2 and C6—H6···O2 hydrogen bonds form a $R_2^1(6)$ graph-set motif. (Fig. 2).

Synthesis and crystallization

The compound was prepared by refluxing a mixture of a solution containing *N*-(3-formylpyridin-2-yl)acetamide (0.20 g, 0.97 mol) in 20 ml ethanol and a solution containing 5-amino-2-methylphenol (0.12 g, 0.97 mol) in 20 ml ethanol. The reaction mixture was stirred for 1 h under reflux. Crystals of *N*-(3-{[(*Z*)-(3-Hydroxy-4-methylphenyl)imino]methyl}-pyridin-2-yl)pivalamide suitable for X-ray analysis were obtained from ethyl alcohol by slow evaporation (yield 65%; m.p. 433–435 K).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The three adjacent methyl groups are each disordered over two sets of sites with an occupancy ratio of 0.692 (5):0.308 (5).

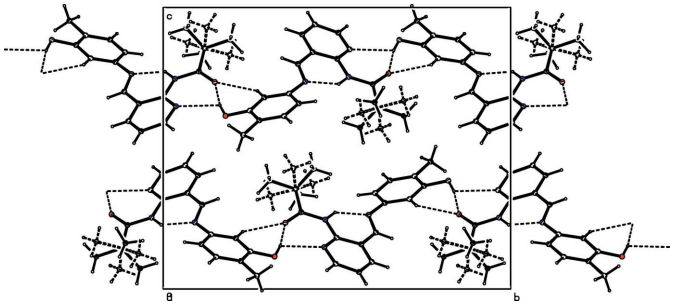


Figure 2
The molecular packing in (I), viewed along the *bc* plane, showing the hydrogen-bonding interactions as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···N1	0.91 (3)	1.94 (3)	2.709 (3)	142 (2)
O1—H1···O2^{i}	0.94 (3)	1.90 (3)	2.827 (3)	169 (3)
C6—H6···O2^{i}	0.93	2.46	3.160 (3)	132
O1—H1···N2^{i}	0.94 (3)	2.42 (3)	2.905 (3)	112 (2)

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{21}N_3O_2$
M_r	311.38
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	5.8594 (3), 18.8756 (8), 16.0649 (9)
β (°)	108.130 (4)
V (Å^3)	1688.56 (15)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.80 × 0.39 × 0.15
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Integration (*X-RED32*; Stoe & Cie, 2002)
T_{min}, T_{max}	0.959, 0.988
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18264, 3133, 1817
R_{int}	0.086
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.059, 0.142, 1.02
No. of reflections	3133
No. of parameters	251
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})	0.23, −0.29

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2002), *SHELXS2013* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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full crystallographic data

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N-(3-{[(*Z*)-(3-Hydroxy-4-methylphenyl)imino]methyl}pyridin-2-yl)pivalamide

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_N_-(3-{[(_Z_)-(3-Hydroxy-4-methylphenyl)imino]methyl}pyridin-2-yl)pivalamide

Crystal data

$C_{18}H_{21}N_3O_2$
M_r = 311.38
Monoclinic, $P2_1/c$
a = 5.8594 (3) Å
b = 18.8756 (8) Å
c = 16.0649 (9) Å
β = 108.130 (4)°
V = 1688.56 (15) Å^3
Z = 4
$F(000)$ = 664
D_x = 1.225 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 14515 reflections
θ = 1.7–28.0°
μ = 0.08 mm^{-1}
T = 296 K
Prism, brown
0.80 × 0.39 × 0.15 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
w scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.959, T_{max} = 0.988
18264 measured reflections
3133 independent reflections
1817 reflections with $I > 2\sigma(I)$
R_{int} = 0.086
θ_{max} = 25.5°, θ_{min} = 1.7°
h = −7→6
k = −22→22
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.142
S = 1.02
3133 reflections
251 parameters
127 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.8358 (4)	0.17960 (10)	0.61515 (14)	0.0865 (6)	
H1	0.747 (5)	0.1641 (17)	0.651 (2)	0.106 (11)*	
O2	0.4154 (4)	0.64845 (9)	0.76485 (12)	0.0820 (6)	
N1	0.7248 (4)	0.40900 (10)	0.73668 (13)	0.0617 (5)	
N2	0.2929 (4)	0.53625 (11)	0.85112 (14)	0.0719 (6)	
N3	0.5143 (4)	0.53363 (11)	0.75354 (13)	0.0643 (6)	
H3	0.596 (4)	0.5043 (15)	0.7283 (16)	0.080 (8)*	
C1	1.1789 (5)	0.23035 (16)	0.54733 (19)	0.0840 (8)	
H1A	1.2982	0.2569	0.5311	0.126*	
H1B	1.0578	0.2142	0.4955	0.126*	
H1C	1.2530	0.1903	0.5821	0.126*	
C2	1.0658 (4)	0.27668 (13)	0.59944 (15)	0.0620 (6)	
C3	1.1226 (4)	0.34738 (15)	0.61428 (17)	0.0692 (7)	
H3A	1.2396	0.3667	0.5931	0.083*	
C4	1.0117 (4)	0.39038 (14)	0.65947 (16)	0.0669 (7)	
H4	1.0507	0.4382	0.6668	0.080*	
C5	0.8425 (4)	0.36226 (12)	0.69392 (15)	0.0578 (6)	
C6	0.7827 (4)	0.29104 (13)	0.68071 (16)	0.0632 (7)	
H6	0.6689	0.2715	0.7034	0.076*	
C7	0.8929 (4)	0.24909 (13)	0.63352 (16)	0.0621 (6)	
C8	0.6531 (5)	0.38784 (13)	0.79951 (16)	0.0659 (7)	
H8	0.6945	0.3421	0.8204	0.079*	
C9	0.5106 (5)	0.43017 (13)	0.84111 (15)	0.0614 (6)	
C10	0.4257 (6)	0.39989 (15)	0.90404 (17)	0.0798 (8)	
H10	0.4710	0.3539	0.9227	0.096*	
C11	0.2756 (6)	0.43647 (16)	0.93950 (19)	0.0860 (9)	
H11	0.2184	0.4161	0.9818	0.103*	
C12	0.2138 (5)	0.50374 (15)	0.91025 (18)	0.0797 (8)	
H12	0.1096	0.5285	0.9331	0.096*	
C13	0.4383 (4)	0.50074 (13)	0.81772 (15)	0.0587 (6)	
C14	0.4893 (4)	0.60268 (12)	0.72722 (15)	0.0582 (6)	
C15	0.5581 (4)	0.61932 (12)	0.64528 (16)	0.0689 (7)	
C16A	0.4632 (13)	0.6921 (3)	0.6128 (4)	0.116 (2)	0.692 (5)
H16A	0.5498	0.7273	0.6537	0.174*	0.692 (5)
H16B	0.2956	0.6947	0.6076	0.174*	0.692 (5)
H16C	0.4839	0.7005	0.5567	0.174*	0.692 (5)
C17A	0.8202 (8)	0.6085 (4)	0.6612 (4)	0.118 (2)	0.692 (5)
H17A	0.8624	0.5606	0.6798	0.178*	0.692 (5)
H17B	0.9093	0.6406	0.7059	0.178*	0.692 (5)
H17C	0.8578	0.6174	0.6081	0.178*	0.692 (5)
C18A	0.4119 (11)	0.5685 (3)	0.5722 (3)	0.1133 (19)	0.692 (5)
H18A	0.4248	0.5836	0.5168	0.170*	0.692 (5)
H18B	0.2464	0.5691	0.5701	0.170*	0.692 (5)
H18C	0.4742	0.5213	0.5845	0.170*	0.692 (5)
C16B	0.707 (3)	0.6891 (5)	0.6645 (7)	0.108 (3)	0.308 (5)

H16D	0.8546	0.6810	0.7109	0.162*	0.308 (5)
H16E	0.6166	0.7254	0.6819	0.162*	0.308 (5)
H16F	0.7428	0.7039	0.6127	0.162*	0.308 (5)
C17B	0.744 (2)	0.5694 (6)	0.6318 (8)	0.095 (3)	0.308 (5)
H17D	0.8087	0.5886	0.5886	0.142*	0.308 (5)
H17E	0.6710	0.5243	0.6122	0.142*	0.308 (5)
H17F	0.8708	0.5634	0.6861	0.142*	0.308 (5)
C18B	0.3418 (18)	0.6264 (10)	0.5670 (5)	0.120 (3)	0.308 (5)
H18D	0.2282	0.6575	0.5803	0.180*	0.308 (5)
H18E	0.2700	0.5806	0.5509	0.180*	0.308 (5)
H18F	0.3876	0.6456	0.5192	0.180*	0.308 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1293 (17)	0.0495 (11)	0.1086 (15)	−0.0107 (10)	0.0777 (14)	−0.0129 (10)
O2	0.1252 (15)	0.0484 (11)	0.0981 (14)	0.0045 (10)	0.0722 (12)	0.0004 (10)
N1	0.0746 (13)	0.0457 (12)	0.0685 (13)	0.0012 (10)	0.0275 (11)	−0.0028 (10)
N2	0.0971 (15)	0.0585 (14)	0.0741 (14)	0.0062 (11)	0.0471 (13)	0.0044 (11)
N3	0.0950 (15)	0.0451 (12)	0.0655 (13)	0.0088 (11)	0.0434 (12)	0.0055 (10)
C1	0.099 (2)	0.080 (2)	0.090 (2)	0.0062 (16)	0.0536 (17)	−0.0020 (15)
C2	0.0703 (15)	0.0580 (16)	0.0630 (15)	0.0034 (12)	0.0286 (13)	0.0032 (12)
C3	0.0684 (16)	0.0683 (18)	0.0783 (17)	−0.0067 (13)	0.0333 (14)	0.0015 (14)
C4	0.0729 (16)	0.0518 (15)	0.0773 (17)	−0.0084 (12)	0.0253 (14)	−0.0008 (13)
C5	0.0654 (14)	0.0474 (14)	0.0624 (15)	−0.0005 (11)	0.0224 (12)	−0.0009 (11)
C6	0.0771 (16)	0.0497 (15)	0.0736 (16)	−0.0019 (12)	0.0389 (13)	−0.0006 (12)
C7	0.0813 (16)	0.0440 (14)	0.0684 (15)	−0.0011 (12)	0.0340 (13)	−0.0012 (12)
C8	0.0918 (18)	0.0422 (14)	0.0645 (15)	0.0006 (12)	0.0256 (14)	0.0013 (12)
C9	0.0904 (18)	0.0435 (14)	0.0542 (14)	−0.0025 (12)	0.0280 (13)	−0.0019 (11)
C10	0.128 (2)	0.0491 (16)	0.0721 (17)	−0.0036 (16)	0.0451 (17)	0.0043 (13)
C11	0.132 (2)	0.0627 (18)	0.0846 (19)	−0.0134 (17)	0.0640 (19)	0.0019 (15)
C12	0.106 (2)	0.0656 (19)	0.0868 (19)	−0.0013 (15)	0.0578 (17)	−0.0007 (15)
C13	0.0792 (15)	0.0483 (15)	0.0533 (13)	−0.0037 (12)	0.0275 (12)	−0.0016 (11)
C14	0.0722 (15)	0.0462 (14)	0.0617 (14)	−0.0002 (11)	0.0288 (12)	−0.0027 (11)
C15	0.0938 (17)	0.0585 (15)	0.0668 (15)	0.0089 (12)	0.0431 (13)	0.0094 (12)
C16A	0.176 (5)	0.091 (3)	0.113 (4)	0.046 (3)	0.090 (4)	0.049 (3)
C17A	0.085 (3)	0.151 (5)	0.133 (5)	−0.002 (3)	0.056 (3)	0.046 (4)
C18A	0.156 (4)	0.131 (4)	0.056 (2)	−0.018 (4)	0.038 (3)	−0.003 (3)
C16B	0.156 (7)	0.093 (5)	0.100 (6)	−0.027 (5)	0.073 (5)	0.013 (5)
C17B	0.106 (6)	0.109 (6)	0.097 (6)	−0.002 (5)	0.072 (5)	0.023 (5)
C18B	0.132 (6)	0.145 (8)	0.083 (5)	0.014 (6)	0.033 (5)	0.036 (6)

Geometric parameters (Å, º)

O1—C7	1.363 (3)	C11—C12	1.363 (4)
O1—H1	0.94 (3)	C11—H11	0.9300
O2—C14	1.209 (3)	C12—H12	0.9300
N1—C8	1.272 (3)	C14—C15	1.525 (3)

N1—C5	1.421 (3)	C15—C18B	1.488 (6)
N2—C13	1.322 (3)	C15—C17A	1.490 (4)
N2—C12	1.329 (3)	C15—C17B	1.506 (6)
N3—C14	1.364 (3)	C15—C16A	1.512 (4)
N3—C13	1.390 (3)	C15—C18A	1.552 (4)
N3—H3	0.91 (3)	C15—C16B	1.558 (6)
C1—C2	1.500 (3)	C16A—H16A	0.9600
C1—H1A	0.9600	C16A—H16B	0.9600
C1—H1B	0.9600	C16A—H16C	0.9600
C1—H1C	0.9600	C17A—H17A	0.9600
C2—C3	1.378 (3)	C17A—H17B	0.9600
C2—C7	1.394 (3)	C17A—H17C	0.9600
C3—C4	1.379 (3)	C18A—H18A	0.9600
C3—H3A	0.9300	C18A—H18B	0.9600
C4—C5	1.383 (3)	C18A—H18C	0.9600
C4—H4	0.9300	C16B—H16D	0.9600
C5—C6	1.389 (3)	C16B—H16E	0.9600
C6—C7	1.387 (3)	C16B—H16F	0.9600
C6—H6	0.9300	C17B—H17D	0.9600
C8—C9	1.459 (3)	C17B—H17E	0.9600
C8—H8	0.9300	C17B—H17F	0.9600
C9—C10	1.382 (3)	C18B—H18D	0.9600
C9—C13	1.413 (3)	C18B—H18E	0.9600
C10—C11	1.373 (4)	C18B—H18F	0.9600
C10—H10	0.9300		

C7—O1—H1	108 (2)	N3—C14—C15	115.6 (2)
C8—N1—C5	121.2 (2)	C18B—C15—C17B	113.5 (8)
C13—N2—C12	117.9 (2)	C17A—C15—C16A	115.6 (4)
C14—N3—C13	128.9 (2)	C18B—C15—C14	111.3 (4)
C14—N3—H3	117.8 (17)	C17A—C15—C14	111.1 (3)
C13—N3—H3	113.2 (17)	C17B—C15—C14	113.1 (4)
C2—C1—H1A	109.5	C16A—C15—C14	108.5 (2)
C2—C1—H1B	109.5	C17A—C15—C18A	110.0 (4)
H1A—C1—H1B	109.5	C16A—C15—C18A	104.1 (4)
C2—C1—H1C	109.5	C14—C15—C18A	107.1 (2)
H1A—C1—H1C	109.5	C18B—C15—C16B	111.7 (8)
H1B—C1—H1C	109.5	C17B—C15—C16B	99.9 (8)
C3—C2—C7	117.4 (2)	C14—C15—C16B	106.6 (3)
C3—C2—C1	122.4 (2)	C15—C16A—H16A	109.5
C7—C2—C1	120.2 (2)	C15—C16A—H16B	109.5
C2—C3—C4	122.2 (2)	H16A—C16A—H16B	109.5
C2—C3—H3A	118.9	C15—C16A—H16C	109.5
C4—C3—H3A	118.9	H16A—C16A—H16C	109.5
C3—C4—C5	119.9 (2)	H16B—C16A—H16C	109.5
C3—C4—H4	120.0	C15—C17A—H17A	109.5
C5—C4—H4	120.0	C15—C17A—H17B	109.5
C4—C5—C6	119.2 (2)	H17A—C17A—H17B	109.5

C4—C5—N1	118.1 (2)	C15—C17A—H17C	109.5
C6—C5—N1	122.5 (2)	H17A—C17A—H17C	109.5
C7—C6—C5	119.9 (2)	H17B—C17A—H17C	109.5
C7—C6—H6	120.1	C15—C18A—H18A	109.5
C5—C6—H6	120.1	C15—C18A—H18B	109.5
O1—C7—C6	122.9 (2)	H18A—C18A—H18B	109.5
O1—C7—C2	115.7 (2)	C15—C18A—H18C	109.5
C6—C7—C2	121.4 (2)	H18A—C18A—H18C	109.5
N1—C8—C9	124.7 (2)	H18B—C18A—H18C	109.5
N1—C8—H8	117.7	C15—C16B—H16D	109.5
C9—C8—H8	117.7	C15—C16B—H16E	109.5
C10—C9—C13	116.0 (2)	H16D—C16B—H16E	109.5
C10—C9—C8	119.7 (2)	C15—C16B—H16F	109.5
C13—C9—C8	124.2 (2)	H16D—C16B—H16F	109.5
C11—C10—C9	121.2 (3)	H16E—C16B—H16F	109.5
C11—C10—H10	119.4	C15—C17B—H17D	109.5
C9—C10—H10	119.4	C15—C17B—H17E	109.5
C12—C11—C10	117.5 (3)	H17D—C17B—H17E	109.5
C12—C11—H11	121.3	C15—C17B—H17F	109.5
C10—C11—H11	121.3	H17D—C17B—H17F	109.5
N2—C12—C11	124.2 (3)	H17E—C17B—H17F	109.5
N2—C12—H12	117.9	C15—C18B—H18D	109.5
C11—C12—H12	117.9	C15—C18B—H18E	109.5
N2—C13—N3	118.0 (2)	H18D—C18B—H18E	109.5
N2—C13—C9	123.2 (2)	C15—C18B—H18F	109.5
N3—C13—C9	118.7 (2)	H18D—C18B—H18F	109.5
O2—C14—N3	123.3 (2)	H18E—C18B—H18F	109.5
O2—C14—C15	121.1 (2)		

C7—C2—C3—C4	−1.2 (4)	C12—N2—C13—N3	177.7 (2)
C1—C2—C3—C4	177.6 (2)	C12—N2—C13—C9	0.7 (4)
C2—C3—C4—C5	2.0 (4)	C14—N3—C13—N2	10.6 (4)
C3—C4—C5—C6	−1.4 (4)	C14—N3—C13—C9	−172.3 (2)
C3—C4—C5—N1	−177.3 (2)	C10—C9—C13—N2	−1.9 (4)
C8—N1—C5—C4	−149.3 (2)	C8—C9—C13—N2	174.2 (2)
C8—N1—C5—C6	35.0 (3)	C10—C9—C13—N3	−178.8 (2)
C4—C5—C6—C7	0.1 (4)	C8—C9—C13—N3	−2.7 (4)
N1—C5—C6—C7	175.8 (2)	C13—N3—C14—O2	8.5 (4)
C5—C6—C7—O1	−177.3 (2)	C13—N3—C14—C15	−170.8 (2)
C5—C6—C7—C2	0.7 (4)	O2—C14—C15—C18B	−77.5 (8)
C3—C2—C7—O1	178.0 (2)	N3—C14—C15—C18B	101.8 (8)
C1—C2—C7—O1	−0.8 (3)	O2—C14—C15—C17A	114.9 (4)
C3—C2—C7—C6	−0.2 (4)	N3—C14—C15—C17A	−65.8 (4)
C1—C2—C7—C6	−178.9 (2)	O2—C14—C15—C17B	153.3 (7)
C5—N1—C8—C9	−173.7 (2)	N3—C14—C15—C17B	−27.4 (7)
N1—C8—C9—C10	174.7 (2)	O2—C14—C15—C16A	−13.2 (4)
N1—C8—C9—C13	−1.3 (4)	N3—C14—C15—C16A	166.1 (4)
C13—C9—C10—C11	1.5 (4)	O2—C14—C15—C18A	−125.0 (4)

C8—C9—C10—C11	−174.8 (3)	N3—C14—C15—C18A	54.3 (4)
C9—C10—C11—C12	0.0 (4)	O2—C14—C15—C16B	44.6 (7)
C13—N2—C12—C11	0.9 (4)	N3—C14—C15—C16B	−136.1 (7)
C10—C11—C12—N2	−1.3 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···N1	0.91 (3)	1.94 (3)	2.709 (3)	142 (2)
O1—H1···O2^{i}	0.94 (3)	1.90 (3)	2.827 (3)	169 (3)
C6—H6···O2^{i}	0.93	2.46	3.160 (3)	132
O1—H1···N2^{i}	0.94 (3)	2.42 (3)	2.905 (3)	112 (2)

Symmetry code: (i) −*x*+1, *y*−1/2, −*z*+3/2.