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Crystal structure of dimethyl[(*E*)-2-(1-methyl-5-nitro-1*H*-imidazol-4-yl)ethenyl]amine

Nikolai Beliaev[a]* and Pavel Slepukhin[b]

[a]Ural Federal University, Mira 19 Ekaterinburg 620002, Russian Federation, and [b]Postovsky Institute of Organic Synthesis, Kovalevskoy 22 Ekaterinburg 620090, Russian Federation. *Correspondence e-mail: n.a.beliaev@urfu.ru

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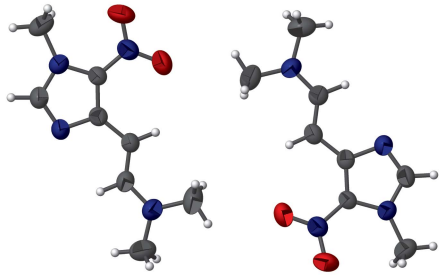
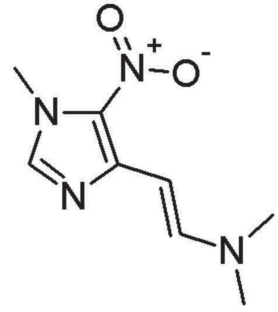
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_8H_{12}N_4O_2$, crystallized with two independent molecules in the asymmetric unit. The bonds lengths of the enamine moiety show strong conjugation in the N—C═C system. In the crystal, the two independent molecules are linked by C—H···O hydrogen bonds, forming zigzag chains along [10$\bar{1}$]. The chains are linked by further C—H···O hydrogen bonds, forming layers parallel to the *ac* plane.

3D view



Chemical scheme



Structure description

The title enamine was synthesized for the study of the [3 + 2] cycloaddition reactions with azides (Bakulev *et al.*, 2012) and hydroxamoylchlorides (Bakulev *et al.*, 2013). It crystallized with two independent molecules in the asymmetric unit, Fig. 1. Both molecules are relatively planar. The mean plane of the *N*,*N*-dimethylethenamine group N2/C3/C6–C8 is inclined to the imidazole ring N1/N3/C1/C4/C5 by 2.16 (11)°, while the mean plane of the *N*,*N*-dimethylethenamine group N2*A*/C3*A*/C6*A*–C8*A* is inclined to the imidazole ring N*A*1/N3*A*/C1*A*/C4*A*/C5*A* by 6.17 (12)°. The NO_2 group is inclined to the imidazole ring by 8.2 (2)° for ring N1/N3/C1/C4/C5 *vs*. N4/O1/O2, and 5.0 (2)° for ring N1*A*/N3*A*/C1*A*/C4*A*/C5*A* *vs*. N4*A*/O1*A*/O2*A*. The substituents at the C3═C8 and C3*A*═C8*A* bonds are placed in *trans*-positions. The bonds lengths of the enamine moiety show strong conjugation in the N—C=C system. The N—C bond lengths and C═C bond lengths in the two molecules are very similar: N2—C8 is 1.326 (2) and N2*A*—C8*A* 1.331 (2) Å, and C8═C3 is 1.342 (3) and C8*A*═C3*A* is 1.334 (2) Å.

In the crystal, the two independent molecules are linked by C—H···O hydrogen bonds, forming zigzag chains along [10$\bar{1}$]. The chains are linked by further C—H···O hydrogen bonds, forming layers parallel to the *ac* plane; see Fig. 2 and Table 1.

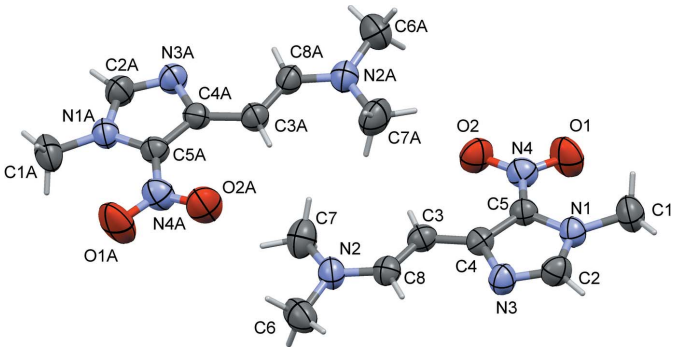


Figure 1
A view of the molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

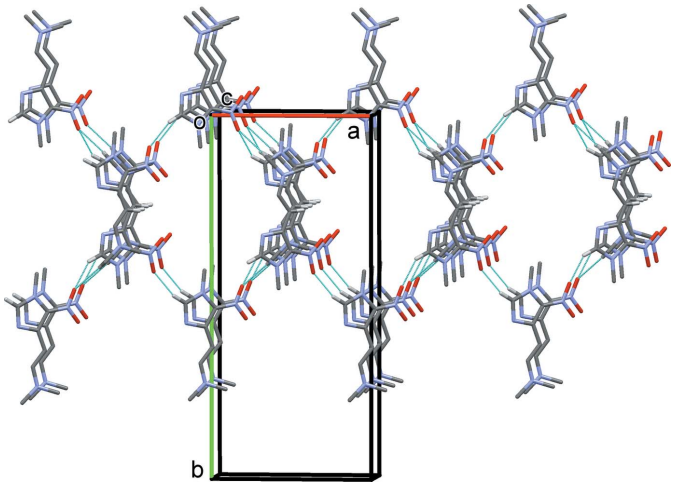


Figure 2
A view along the *c* axis of the crystal packing of the title compound. Hydrogen bonds are drawn as dashed lines (see Table 1), and H atoms not involved in these interactions have been omitted for clarity.

Synthesis and crystallization

The title compound was synthesized from 1,4-dimethyl-5-nitro-1*H*-imidazole following a reported procedure (Hosmane *et al.*, 1985), illustrated in Fig. 3, and crystallized from ethanol yielding dark-red prismatic crystals.

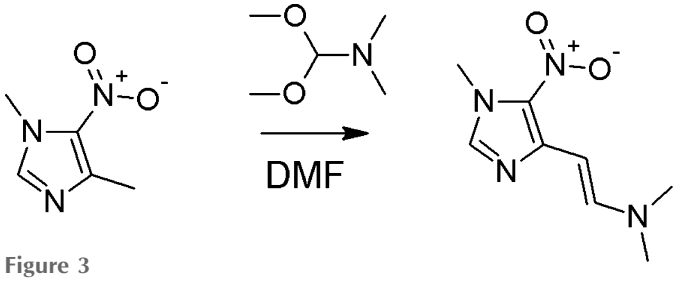


Figure 3
Reaction scheme.

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1A^{i}	0.954 (15)	2.399 (15)	3.235 (3)	146 (1)
C2A—H2A···O1^{ii}	0.958 (16)	2.254 (15)	3.181 (3)	162 (1)
C6—H6B···O1A^{iii}	0.96	2.58	3.461 (3)	153

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_8H_{12}N_4O_2$
M_r	196.22
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, b, c (Å)	10.5015 (12), 23.561 (3), 7.7533 (6)
β (°)	96.604 (8)
V (Å^3)	1905.6 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.25 × 0.20 × 0.15
Data collection	
Diffractometer	Oxford Diffraction Xcalibur S CCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10647, 3875, 1523
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.066, 1.00
No. of reflections	3875
No. of parameters	284
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.14, −0.12

Computer programs: *CrysAlis CCD* (Oxford Diffraction, 2006), *CrysAlis RED* (Oxford Diffraction, 2006), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x152488 [doi:10.1107/S2414314615024888]

Crystal structure of dimethyl[(*E*)-2-(1-methyl-5-nitro-1*H*-imidazol-4-yl)ethenyl]amine

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Dimethyl[(*E*)-2-(1-methyl-5-nitro-1*H*-imidazol-4-yl)ethenyl]amine

Crystal data

$C_8H_{12}N_4O_2$
M_r = 196.22
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 10.5015 (12) Å
b = 23.561 (3) Å
c = 7.7533 (6) Å
β = 96.604 (8)°
V = 1905.6 (3) Å^3
Z = 8
$F(000)$ = 832
D_x = 1.368 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1523 reflections
θ = 2.8–26.4°
μ = 0.10 mm^{-1}
T = 295 K
Prism, red
0.25 × 0.20 × 0.15 mm

Data collection

Oxford Diffraction Xcalibur S CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
10647 measured reflections
3875 independent reflections
1523 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.4°, θ_{min} = 2.8°
h = −13→13
k = −28→29
l = −9→6

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.066
S = 1.00
3875 reflections
284 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
$w = 1/[\sigma^2(F_o^2) + (0.016P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00217 (15)

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.

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 $F^2 > \sigma(F^2)$ 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}
N1	0.44977 (16)	0.40312 (6)	0.2065 (2)	0.0497 (5)
N1A	1.04292 (17)	−0.01495 (7)	0.7905 (2)	0.0531 (5)
O1A	0.80215 (14)	−0.03162 (6)	0.6211 (2)	0.0983 (6)
C1A	1.02942 (19)	−0.07638 (7)	0.7864 (2)	0.0718 (6)
H1AA	1.1008	−0.0933	0.8564	0.108*
H1AB	1.0273	−0.0895	0.6689	0.108*
H1AC	0.9512	−0.0869	0.8312	0.108*
O2A	0.78287 (14)	0.05713 (6)	0.56123 (18)	0.0818 (5)
N2A	1.02826 (16)	0.23407 (8)	0.7367 (2)	0.0608 (5)
C2A	1.1448 (2)	0.01246 (9)	0.8654 (3)	0.0615 (6)
N3A	1.14002 (15)	0.06755 (7)	0.8499 (2)	0.0587 (5)
C3A	0.9826 (2)	0.13453 (8)	0.7150 (3)	0.0510 (6)
C4A	1.02459 (18)	0.07855 (7)	0.7556 (2)	0.0454 (5)
N4A	0.84503 (18)	0.01685 (7)	0.6297 (2)	0.0619 (5)
C5A	0.96365 (19)	0.02736 (8)	0.7181 (2)	0.0471 (5)
C6A	1.12128 (19)	0.27801 (8)	0.7863 (3)	0.0796 (7)
H6AA	1.1992	0.2611	0.8394	0.119*
H6AB	1.0881	0.3033	0.8672	0.119*
H6AC	1.1384	0.2988	0.6850	0.119*
C7A	0.9047 (2)	0.25138 (8)	0.6542 (3)	0.0795 (8)
H7AA	0.8388	0.2348	0.7140	0.119*
H7AB	0.8947	0.2389	0.5355	0.119*
H7AC	0.8981	0.2920	0.6580	0.119*
C8A	1.0565 (2)	0.17934 (9)	0.7605 (3)	0.0511 (6)
O1	0.66579 (13)	0.42352 (6)	0.43092 (17)	0.0828 (5)
C1	0.46003 (19)	0.46466 (8)	0.2120 (2)	0.0690 (7)
H1A	0.3908	0.4810	0.1365	0.104*
H1B	0.5402	0.4760	0.1745	0.104*
H1C	0.4559	0.4776	0.3286	0.104*
O2	0.71826 (12)	0.33445 (6)	0.43022 (17)	0.0716 (4)
N2	0.49194 (15)	0.15456 (7)	0.21675 (19)	0.0565 (5)
C2	0.3544 (2)	0.37399 (10)	0.1211 (3)	0.0557 (6)
N3	0.36672 (15)	0.31899 (7)	0.12659 (19)	0.0540 (5)
C3	0.5290 (2)	0.25429 (8)	0.2591 (3)	0.0490 (6)
C4	0.48305 (17)	0.30967 (7)	0.2234 (2)	0.0436 (5)

N4	0.64519 (17)	0.37394 (7)	0.3824 (2)	0.0553 (5)
C5	0.53483 (19)	0.36189 (8)	0.2743 (2)	0.0440 (5)
C6	0.4020 (2)	0.11081 (8)	0.1539 (3)	0.0760 (7)
H6A	0.3369	0.1268	0.0710	0.114*
H6B	0.3630	0.0952	0.2495	0.114*
H6C	0.4463	0.0813	0.0995	0.114*
C7	0.60698 (19)	0.13755 (8)	0.3232 (2)	0.0726 (7)
H7A	0.6803	0.1529	0.2759	0.109*
H7B	0.6125	0.0969	0.3254	0.109*
H7C	0.6049	0.1515	0.4391	0.109*
C8	0.4624 (2)	0.20899 (9)	0.1940 (3)	0.0494 (6)
H2	0.2798 (15)	0.3923 (6)	0.0652 (19)	0.048 (5)*
H2A	1.2150 (16)	−0.0078 (6)	0.927 (2)	0.064 (6)*
H8A	1.1417 (15)	0.1740 (6)	0.8116 (19)	0.057 (6)*
H3A	0.9011 (15)	0.1399 (6)	0.6555 (19)	0.054 (6)*
H8	0.3814 (15)	0.2149 (6)	0.1173 (19)	0.049 (5)*
H3	0.6049 (15)	0.2509 (6)	0.3238 (19)	0.053 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0538 (11)	0.0434 (11)	0.0506 (11)	0.0017 (10)	0.0003 (9)	0.0025 (9)
N1A	0.0560 (12)	0.0434 (11)	0.0594 (12)	0.0008 (10)	0.0038 (10)	0.0030 (9)
O1A	0.0962 (13)	0.0684 (10)	0.1209 (14)	−0.0340 (9)	−0.0282 (10)	0.0003 (10)
C1A	0.0934 (17)	0.0440 (14)	0.0788 (16)	−0.0007 (12)	0.0138 (13)	0.0044 (13)
O2A	0.0665 (10)	0.0818 (11)	0.0895 (12)	−0.0025 (9)	−0.0231 (9)	0.0131 (9)
N2A	0.0581 (13)	0.0494 (12)	0.0741 (13)	0.0052 (10)	0.0046 (11)	0.0024 (10)
C2A	0.0515 (15)	0.0555 (16)	0.0745 (17)	0.0045 (13)	−0.0050 (13)	0.0077 (14)
N3A	0.0482 (11)	0.0517 (11)	0.0727 (12)	0.0015 (9)	−0.0082 (9)	0.0051 (10)
C3A	0.0460 (16)	0.0481 (15)	0.0568 (15)	0.0001 (12)	−0.0038 (13)	0.0024 (11)
C4A	0.0420 (13)	0.0476 (13)	0.0464 (13)	−0.0023 (11)	0.0045 (11)	0.0032 (11)
N4A	0.0610 (14)	0.0622 (13)	0.0594 (13)	−0.0089 (11)	−0.0062 (11)	0.0008 (11)
C5A	0.0440 (13)	0.0477 (14)	0.0483 (14)	−0.0026 (12)	−0.0003 (11)	0.0006 (11)
C6A	0.0816 (17)	0.0568 (15)	0.1014 (18)	−0.0096 (13)	0.0145 (15)	−0.0051 (13)
C7A	0.0725 (18)	0.0775 (18)	0.0875 (17)	0.0255 (13)	0.0043 (15)	0.0161 (13)
C8A	0.0484 (15)	0.0473 (15)	0.0570 (15)	0.0094 (12)	0.0035 (12)	0.0023 (12)
O1	0.0893 (12)	0.0601 (9)	0.0920 (12)	−0.0178 (8)	−0.0203 (9)	−0.0156 (9)
C1	0.0809 (16)	0.0462 (14)	0.0779 (16)	0.0007 (11)	0.0001 (13)	0.0059 (12)
O2	0.0562 (9)	0.0739 (10)	0.0796 (10)	0.0090 (8)	−0.0139 (8)	−0.0015 (8)
N2	0.0629 (12)	0.0424 (12)	0.0633 (12)	0.0028 (9)	0.0032 (10)	0.0003 (10)
C2	0.0483 (15)	0.0629 (16)	0.0535 (15)	0.0034 (13)	−0.0048 (12)	0.0048 (13)
N3	0.0531 (11)	0.0482 (11)	0.0583 (11)	0.0049 (8)	−0.0036 (9)	0.0007 (9)
C3	0.0437 (15)	0.0555 (16)	0.0470 (14)	0.0015 (12)	0.0013 (12)	−0.0002 (12)
C4	0.0455 (14)	0.0485 (13)	0.0363 (12)	0.0022 (11)	0.0030 (10)	0.0028 (11)
N4	0.0538 (12)	0.0571 (13)	0.0534 (12)	−0.0025 (10)	0.0000 (10)	−0.0006 (10)
C5	0.0425 (13)	0.0466 (14)	0.0413 (13)	−0.0020 (11)	−0.0014 (11)	−0.0022 (11)
C6	0.0903 (18)	0.0578 (15)	0.0823 (16)	−0.0160 (13)	0.0199 (15)	−0.0092 (13)
C7	0.0865 (18)	0.0634 (16)	0.0663 (15)	0.0184 (12)	0.0015 (14)	0.0055 (12)

C8	0.0527 (15)	0.0493 (15)	0.0463 (14)	0.0022 (12)	0.0061 (12)	−0.0010 (11)

Geometric parameters (Å, º)

N1—C2	1.327 (2)	C7A—H7AB	0.9600
N1—C5	1.382 (2)	C7A—H7AC	0.9600
N1—C1	1.4543 (19)	C8A—H8A	0.944 (14)
N1A—C2A	1.325 (2)	O1—N4	1.2387 (17)
N1A—C5A	1.376 (2)	C1—H1A	0.9600
N1A—C1A	1.4544 (19)	C1—H1B	0.9600
O1A—N4A	1.2264 (17)	C1—H1C	0.9600
C1A—H1AA	0.9600	O2—N4	1.2355 (17)
C1A—H1AB	0.9600	N2—C8	1.326 (2)
C1A—H1AC	0.9600	N2—C7	1.4393 (19)
O2A—N4A	1.2365 (17)	N2—C6	1.444 (2)
N2A—C8A	1.331 (2)	C2—N3	1.303 (2)
N2A—C7A	1.438 (2)	C2—H2	0.954 (14)
N2A—C6A	1.445 (2)	N3—C4	1.3760 (19)
C2A—N3A	1.304 (2)	C3—C8	1.342 (2)
C2A—H2A	0.959 (15)	C3—C4	1.408 (2)
N3A—C4A	1.3665 (19)	C3—H3	0.895 (14)
C3A—C8A	1.334 (2)	C4—C5	1.384 (2)
C3A—C4A	1.415 (2)	N4—C5	1.379 (2)
C3A—H3A	0.933 (14)	C6—H6A	0.9600
C4A—C5A	1.380 (2)	C6—H6B	0.9600
N4A—C5A	1.374 (2)	C6—H6C	0.9600
C6A—H6AA	0.9600	C7—H7A	0.9600
C6A—H6AB	0.9600	C7—H7B	0.9600
C6A—H6AC	0.9600	C7—H7C	0.9600
C7A—H7AA	0.9600	C8—H8	0.990 (14)
C2—N1—C5	104.14 (17)	N2A—C8A—C3A	128.1 (2)
C2—N1—C1	125.41 (17)	N2A—C8A—H8A	111.9 (9)
C5—N1—C1	130.33 (17)	C3A—C8A—H8A	120.0 (9)
C2A—N1A—C5A	104.22 (18)	N1—C1—H1A	109.5
C2A—N1A—C1A	124.50 (17)	N1—C1—H1B	109.5
C5A—N1A—C1A	131.23 (18)	H1A—C1—H1B	109.5
N1A—C1A—H1AA	109.5	N1—C1—H1C	109.5
N1A—C1A—H1AB	109.5	H1A—C1—H1C	109.5
H1AA—C1A—H1AB	109.5	H1B—C1—H1C	109.5
N1A—C1A—H1AC	109.5	C8—N2—C7	120.89 (17)
H1AA—C1A—H1AC	109.5	C8—N2—C6	120.77 (17)
H1AB—C1A—H1AC	109.5	C7—N2—C6	117.89 (17)
C8A—N2A—C7A	120.78 (18)	N3—C2—N1	115.58 (19)
C8A—N2A—C6A	121.61 (18)	N3—C2—H2	122.6 (9)
C7A—N2A—C6A	117.57 (18)	N1—C2—H2	121.8 (9)
N3A—C2A—N1A	115.10 (19)	C2—N3—C4	104.80 (16)
N3A—C2A—H2A	124.1 (10)	C8—C3—C4	120.7 (2)

N1A—C2A—H2A	120.8 (10)	C8—C3—H3	122.0 (10)
C2A—N3A—C4A	105.09 (16)	C4—C3—H3	117.2 (10)
C8A—C3A—C4A	121.5 (2)	N3—C4—C5	107.98 (15)
C8A—C3A—H3A	119.8 (9)	N3—C4—C3	121.21 (17)
C4A—C3A—H3A	118.7 (9)	C5—C4—C3	130.78 (17)
N3A—C4A—C5A	107.95 (15)	O2—N4—O1	122.57 (17)
N3A—C4A—C3A	122.03 (17)	O2—N4—C5	118.48 (17)
C5A—C4A—C3A	130.00 (18)	O1—N4—C5	118.93 (17)
O1A—N4A—O2A	121.28 (18)	N4—C5—N1	123.21 (17)
O1A—N4A—C5A	120.07 (17)	N4—C5—C4	129.14 (18)
O2A—N4A—C5A	118.65 (17)	N1—C5—C4	107.50 (16)
N4A—C5A—N1A	122.98 (18)	N2—C6—H6A	109.5
N4A—C5A—C4A	129.37 (18)	N2—C6—H6B	109.5
N1A—C5A—C4A	107.64 (16)	H6A—C6—H6B	109.5
N2A—C6A—H6AA	109.5	N2—C6—H6C	109.5
N2A—C6A—H6AB	109.5	H6A—C6—H6C	109.5
H6AA—C6A—H6AB	109.5	H6B—C6—H6C	109.5
N2A—C6A—H6AC	109.5	N2—C7—H7A	109.5
H6AA—C6A—H6AC	109.5	N2—C7—H7B	109.5
H6AB—C6A—H6AC	109.5	H7A—C7—H7B	109.5
N2A—C7A—H7AA	109.5	N2—C7—H7C	109.5
N2A—C7A—H7AB	109.5	H7A—C7—H7C	109.5
H7AA—C7A—H7AB	109.5	H7B—C7—H7C	109.5
N2A—C7A—H7AC	109.5	N2—C8—C3	128.0 (2)
H7AA—C7A—H7AC	109.5	N2—C8—H8	112.8 (8)
H7AB—C7A—H7AC	109.5	C3—C8—H8	119.3 (8)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1*A*^{i}	0.954 (15)	2.399 (15)	3.235 (3)	146 (1)
C2*A*—H2*A*···O1^{ii}	0.958 (16)	2.254 (15)	3.181 (3)	162 (1)
C6—H6*B*···O1*A*^{iii}	0.96	2.58	3.461 (3)	153

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) −*x*+2, *y*−1/2, −*z*+3/2; (iii) −*x*+1, −*y*, −*z*+1.