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4-[(1*H*-Imidazol-1-yl)methyl]-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole

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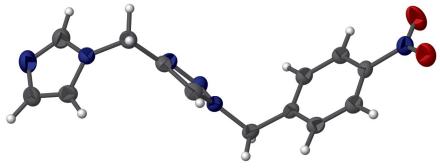
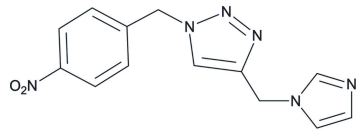
Structural data: full structural data are available from iucrdata.iucr.org

The title molecule, $C_{13}H_{12}N_6O_2$, adopts a slightly twisted zigzag conformation in the crystal, with the dihedral angles between the central triazole ring and the 4-nitrophenyl and imidazole rings being 79.81 (11) and 81.21 (13)°, respectively. The packing features weak C—H···O and C—H···N hydrogen bonds, as well as unusual N═O···π stacking interactions.

3D view



Chemical scheme



Structure description

Triazoles and their derivatives are of great importance in medicinal chemistry and can be used for the synthesis of numerous heterocyclic compounds with different biological activities, including antimicrobial (Sheremet *et al.* 2004), cytotoxic (Sanghvi *et al.*, 1990) and antibacterial activities (Sebbar *et al.*, 2016). They have also been reported to be inhibitors of glycogen synthase kinase-3 (Olesen *et al.*, 2003) and agonists of muscarine receptors (Moltzen *et al.*, 1994). Herein we report the synthesis of 4-[(1*H*-imidazol-1-yl)methyl]-1-(4-nitrobenzyl)-1*H*-1,2,3-triazole by the 1,3-dipolar cycloaddition reaction of 1-(azidomethyl)-4-nitrobenzene with 1-(prop-2-yn-1-yl)-1*H*-imidazole.

The title molecule adopts a slightly twisted, zigzag conformation (Fig. 1) with the dihedral angles between the mean plane of the N2–N4/C8/C9 ring and those of the C1–C6 and N5/N6/C11–C13 rings being, 79.81 (11) and 81.21 (13)°, respectively. The crystal packing features weak C—H···O and C—H···N hydrogen bonds (Table 1, Figs. 2 and 3). In addition, unusual $Cg1\cdots Cg2^{v}$ contacts, where $Cg1$ is the centroid of the C1–C6 ring and $Cg2^{v}$ is the mid-point of the N1═O2 bond [$Cg1\cdots Cg2$ = 2.540 Å; symmetry code: (v) $x, y, z-1$] link molecules into chains along the c-axis direction (Fig. 4). An N—O···π interaction is also observed: O2···$Cg1$ = 3.626 (2) Å, N1···$Cg1$ = 3.5578 (19) Å and N1—O2···$Cg1$ = 77.05 (12)°.

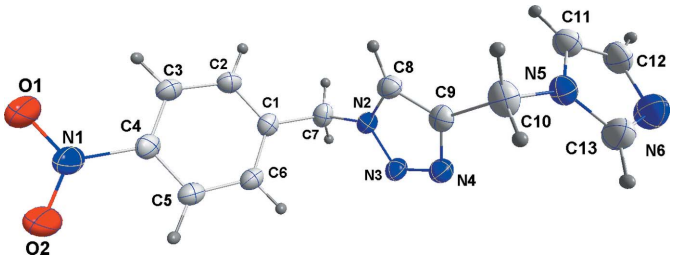


Figure 1
The title molecule with labeling scheme and 50% probability ellipsoids.

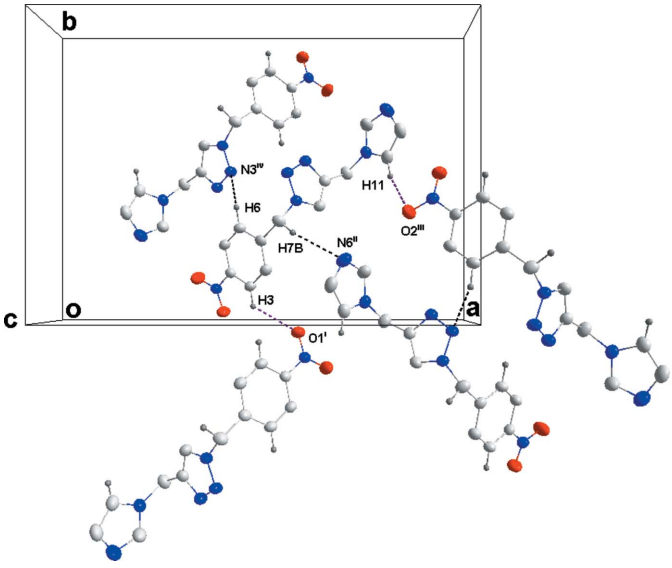


Figure 2
Details of the intermolecular C—H···O and C—H···N hydrogen bonds shown, respectively, as purple and black dashed lines. For symmetry codes see Table 1.

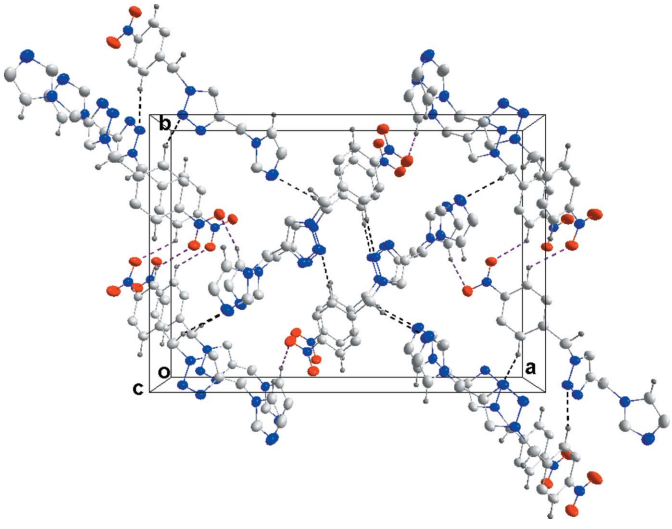


Figure 3
Overall packing viewed along the *c*-axis direction with hydrogen bonds depicted as in Fig. 2.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.98 (2)	2.55 (2)	3.189 (2)	123.0 (18)
C7—H7*B*···N6^{ii}	0.95 (3)	2.60 (3)	3.478 (3)	154 (2)
C11—H11···O2^{iii}	0.98 (3)	2.66 (3)	3.535 (3)	149 (2)
C6—H6···N3^{iv}	1.00 (2)	2.54 (3)	3.299 (3)	133 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{12}N_6O_2$
M_r	284.29
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	150
a, *b*, *c* (Å)	20.3330 (4), 14.2764 (3), 4.5089 (1)
V (Å^3)	1308.85 (5)
Z	4
Radiation type	Cu *Kα*
μ (mm^{-1})	0.86
Crystal size (mm)	0.12 × 0.06 × 0.04
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.88, 0.96
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10013, 2611, 2410
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.029, 0.070, 1.05
No. of reflections	2611
No. of parameters	239
No. of restraints	1
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.12, −0.12
Absolute structure	Flack *x* determined using 956 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.10 (15)

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

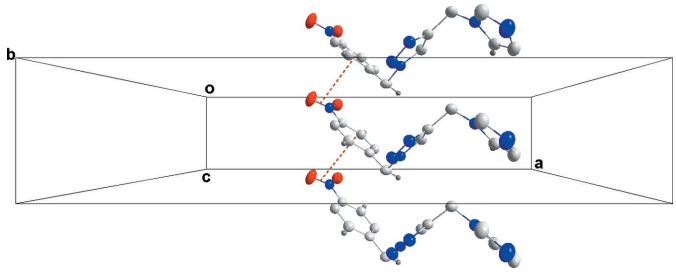


Figure 4
Details of the N═O···π(ring) interactions (dashed lines).

Synthesis and crystallization

In a vial fitted with a screw cap, 1-(azidomethyl)-4-nitrobenzene (100 mg, 0.56 mmol) and 1-(prop-2-yn-1-yl)-1*H*-imidazole (62.5 mg, 0.58 mmol) were added to a mixture of copper(II) sulfate pentahydrate (7 mg, 0.028 mmol), sodium ascorbate (16.6 mg, 0.083 mmol), and β-cyclodextrin (15.9 mg, 0.014 mmol) dissolved in H_2O (1 ml) at room temperature. The reaction mixture was stirred for 15 min at room temperature. The resulting mixture was poured into CH_2Cl_2 (3 ml) and H_2O (3 ml) and the organic layer was separated. The aqueous layer was extracted with CH_2Cl_2 (3 ml) three times. The product was obtained as colorless crystals in 94% yield.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170515 [https://doi.org/10.1107/S2414314617005156]

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Crystal data

$C_{13}H_{12}N_6O_2$
M_r = 284.29
Orthorhombic, $Pna2_1$
a = 20.3330 (4) Å
b = 14.2764 (3) Å
c = 4.5089 (1) Å
V = 1308.85 (5) Å^3
Z = 4
F(000) = 592
D_x = 1.443 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 8050 reflections
θ = 3.8–74.4°
μ = 0.86 mm^{-1}
T = 150 K
Column, colourless
0.12 × 0.06 × 0.04 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.88, T_{max} = 0.96
10013 measured reflections
2611 independent reflections
2410 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 74.5°, θ_{min} = 3.8°
h = −25→23
k = −17→17
l = −5→5

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.070
S = 1.05
2611 reflections
239 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2 + 0.151P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0044 (5)
Absolute structure: Flack x determined using 956 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.10 (15)

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. 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.40535 (8)	0.03081 (10)	0.1143 (4)	0.0449 (4)
O2	0.34070 (8)	0.14915 (12)	0.0656 (6)	0.0567 (5)
N1	0.38941 (8)	0.11157 (12)	0.1721 (4)	0.0344 (4)
N2	0.59199 (8)	0.39660 (11)	0.7619 (4)	0.0284 (3)
N3	0.57204 (8)	0.48647 (12)	0.7668 (5)	0.0339 (4)
N4	0.61097 (8)	0.53343 (11)	0.5897 (4)	0.0335 (4)
N5	0.75335 (8)	0.57154 (12)	0.4154 (4)	0.0327 (4)
N6	0.80031 (10)	0.70206 (14)	0.5784 (6)	0.0528 (5)
H6	0.4522 (12)	0.3802 (17)	0.622 (7)	0.049 (7)*
C1	0.51128 (9)	0.26847 (13)	0.7407 (4)	0.0286 (4)
C2	0.52185 (10)	0.17309 (14)	0.7039 (5)	0.0320 (4)
H2	0.5594 (12)	0.1453 (17)	0.805 (6)	0.038 (6)*
C3	0.48152 (10)	0.12100 (14)	0.5201 (5)	0.0316 (4)
H3	0.4875 (12)	0.0537 (16)	0.492 (6)	0.039 (6)*
C4	0.43084 (9)	0.16574 (13)	0.3753 (4)	0.0285 (4)
C5	0.41831 (10)	0.26072 (13)	0.4096 (5)	0.0311 (4)
H5	0.3822 (13)	0.2882 (17)	0.298 (6)	0.043 (7)*
C6	0.45909 (9)	0.31160 (13)	0.5940 (5)	0.0319 (4)
C7	0.55609 (11)	0.32640 (15)	0.9344 (5)	0.0336 (4)
H7B	0.5873 (12)	0.2880 (16)	1.032 (7)	0.043 (7)*
H7A	0.5293 (12)	0.3618 (17)	1.084 (7)	0.044 (6)*
C8	0.64394 (9)	0.38588 (13)	0.5772 (5)	0.0317 (4)
H8	0.6659 (13)	0.3258 (19)	0.555 (8)	0.054 (7)*
C9	0.65557 (9)	0.47370 (14)	0.4683 (4)	0.0298 (4)
C10	0.70753 (10)	0.50886 (16)	0.2624 (5)	0.0370 (5)
H10A	0.7336 (12)	0.4564 (18)	0.173 (6)	0.048 (7)*
H10B	0.6876 (13)	0.5447 (17)	0.095 (8)	0.052 (7)*
C11	0.80043 (10)	0.54527 (16)	0.6156 (5)	0.0371 (5)
H11	0.8066 (13)	0.4795 (18)	0.667 (6)	0.052 (8)*
C12	0.82835 (11)	0.62560 (17)	0.7119 (6)	0.0436 (5)
H12	0.8633 (14)	0.6326 (19)	0.854 (8)	0.061 (9)*
C13	0.75485 (11)	0.66629 (16)	0.4020 (6)	0.0443 (5)
H13	0.7231 (14)	0.7000 (18)	0.274 (8)	0.059 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0482 (9)	0.0308 (8)	0.0556 (10)	0.0012 (6)	−0.0044 (8)	−0.0094 (7)
O2	0.0456 (9)	0.0427 (9)	0.0819 (14)	0.0054 (7)	−0.0269 (10)	−0.0052 (10)
N1	0.0338 (8)	0.0297 (9)	0.0396 (11)	−0.0019 (7)	−0.0001 (7)	−0.0005 (7)
N2	0.0324 (8)	0.0256 (8)	0.0271 (8)	−0.0006 (6)	−0.0003 (7)	−0.0004 (7)
N3	0.0363 (8)	0.0265 (8)	0.0388 (9)	0.0011 (7)	0.0046 (8)	−0.0026 (8)
N4	0.0355 (8)	0.0289 (8)	0.0361 (9)	0.0012 (7)	0.0019 (8)	0.0007 (8)
N5	0.0309 (8)	0.0378 (9)	0.0294 (8)	−0.0041 (7)	0.0007 (7)	0.0024 (8)
N6	0.0511 (11)	0.0437 (11)	0.0638 (14)	−0.0126 (9)	−0.0085 (11)	0.0014 (11)
C1	0.0319 (9)	0.0278 (9)	0.0260 (9)	−0.0025 (7)	0.0047 (8)	0.0026 (8)
C2	0.0334 (9)	0.0296 (10)	0.0329 (11)	0.0033 (8)	0.0005 (8)	0.0038 (8)
C3	0.0343 (10)	0.0246 (10)	0.0360 (11)	0.0031 (8)	0.0019 (8)	0.0010 (8)
C4	0.0279 (9)	0.0265 (9)	0.0309 (10)	−0.0028 (7)	0.0031 (7)	−0.0001 (8)
C5	0.0310 (9)	0.0277 (10)	0.0345 (10)	0.0049 (8)	0.0007 (9)	0.0015 (9)
C6	0.0356 (9)	0.0242 (9)	0.0359 (10)	0.0022 (8)	0.0018 (9)	0.0009 (8)
C7	0.0418 (11)	0.0319 (10)	0.0270 (10)	−0.0053 (9)	−0.0004 (9)	0.0031 (9)
C8	0.0331 (9)	0.0294 (10)	0.0326 (10)	0.0032 (8)	0.0003 (9)	−0.0041 (9)
C9	0.0325 (9)	0.0307 (10)	0.0262 (10)	−0.0017 (8)	−0.0023 (8)	−0.0035 (8)
C10	0.0376 (11)	0.0449 (12)	0.0284 (10)	−0.0076 (10)	0.0004 (9)	−0.0014 (10)
C11	0.0331 (10)	0.0447 (12)	0.0333 (11)	0.0009 (9)	0.0011 (9)	0.0048 (10)
C12	0.0343 (10)	0.0543 (14)	0.0422 (13)	−0.0087 (10)	−0.0033 (10)	0.0033 (11)
C13	0.0421 (12)	0.0383 (12)	0.0526 (14)	−0.0043 (10)	−0.0047 (11)	0.0062 (12)

Geometric parameters (Å, º)

O1—N1	1.226 (2)	C3—C4	1.377 (3)
O2—N1	1.225 (2)	C3—H3	0.98 (2)
N1—C4	1.465 (3)	C4—C5	1.388 (3)
N2—N3	1.346 (2)	C5—C6	1.381 (3)
N2—C8	1.354 (3)	C5—H5	0.97 (3)
N2—C7	1.464 (3)	C6—H6	1.00 (2)
N3—N4	1.309 (3)	C7—H7B	0.95 (3)
N4—C9	1.360 (3)	C7—H7A	1.00 (3)
N5—C13	1.354 (3)	C8—C9	1.367 (3)
N5—C11	1.368 (3)	C8—H8	0.97 (3)
N5—C10	1.465 (3)	C9—C10	1.493 (3)
N6—C13	1.322 (3)	C10—H10A	1.00 (3)
N6—C12	1.371 (3)	C10—H10B	1.00 (3)
C1—C2	1.389 (3)	C11—C12	1.351 (3)
C1—C6	1.394 (3)	C11—H11	0.98 (3)
C1—C7	1.509 (3)	C12—H12	0.96 (3)
C2—C3	1.383 (3)	C13—H13	0.99 (3)
C2—H2	0.97 (2)		
O2—N1—O1	122.87 (19)	C1—C6—H6	118.7 (16)
O2—N1—C4	118.62 (17)	N2—C7—C1	111.65 (17)

O1—N1—C4	118.51 (16)	N2—C7—H7B	108.0 (15)
N3—N2—C8	110.68 (16)	C1—C7—H7B	110.9 (15)
N3—N2—C7	119.58 (17)	N2—C7—H7A	106.5 (14)
C8—N2—C7	129.69 (17)	C1—C7—H7A	109.7 (14)
N4—N3—N2	107.21 (16)	H7B—C7—H7A	110 (2)
N3—N4—C9	109.13 (16)	N2—C8—C9	104.62 (17)
C13—N5—C11	106.72 (19)	N2—C8—H8	121.6 (18)
C13—N5—C10	127.11 (19)	C9—C8—H8	133.7 (18)
C11—N5—C10	126.05 (19)	N4—C9—C8	108.36 (17)
C13—N6—C12	104.3 (2)	N4—C9—C10	120.75 (18)
C2—C1—C6	119.61 (19)	C8—C9—C10	130.85 (19)
C2—C1—C7	120.89 (18)	N5—C10—C9	111.25 (18)
C6—C1—C7	119.49 (18)	N5—C10—H10A	108.0 (15)
C3—C2—C1	120.49 (19)	C9—C10—H10A	111.9 (15)
C3—C2—H2	121.8 (14)	N5—C10—H10B	107.5 (15)
C1—C2—H2	117.7 (14)	C9—C10—H10B	110.8 (16)
C4—C3—C2	118.59 (18)	H10A—C10—H10B	107 (2)
C4—C3—H3	119.2 (14)	C12—C11—N5	105.9 (2)
C2—C3—H3	122.2 (14)	C12—C11—H11	133.4 (16)
C3—C4—C5	122.51 (19)	N5—C11—H11	120.7 (16)
C3—C4—N1	118.82 (17)	C11—C12—N6	111.1 (2)
C5—C4—N1	118.66 (18)	C11—C12—H12	127.8 (17)
C6—C5—C4	118.09 (19)	N6—C12—H12	121.1 (17)
C6—C5—H5	123.6 (15)	N6—C13—N5	112.0 (2)
C4—C5—H5	118.3 (15)	N6—C13—H13	128.2 (16)
C5—C6—C1	120.70 (18)	N5—C13—H13	119.8 (16)
C5—C6—H6	120.6 (16)		

C8—N2—N3—N4	−0.6 (2)	C2—C1—C7—N2	115.3 (2)
C7—N2—N3—N4	−178.28 (17)	C6—C1—C7—N2	−63.8 (2)
N2—N3—N4—C9	0.6 (2)	N3—N2—C8—C9	0.3 (2)
C6—C1—C2—C3	0.8 (3)	C7—N2—C8—C9	177.69 (19)
C7—C1—C2—C3	−178.38 (18)	N3—N4—C9—C8	−0.5 (2)
C1—C2—C3—C4	0.0 (3)	N3—N4—C9—C10	−178.35 (19)
C2—C3—C4—C5	−0.8 (3)	N2—C8—C9—N4	0.1 (2)
C2—C3—C4—N1	177.84 (17)	N2—C8—C9—C10	177.7 (2)
O2—N1—C4—C3	173.1 (2)	C13—N5—C10—C9	−102.5 (3)
O1—N1—C4—C3	−7.5 (3)	C11—N5—C10—C9	73.0 (3)
O2—N1—C4—C5	−8.2 (3)	N4—C9—C10—N5	65.4 (2)
O1—N1—C4—C5	171.22 (19)	C8—C9—C10—N5	−112.0 (2)
C3—C4—C5—C6	0.8 (3)	C13—N5—C11—C12	−0.4 (2)
N1—C4—C5—C6	−177.84 (19)	C10—N5—C11—C12	−176.6 (2)
C4—C5—C6—C1	0.0 (3)	N5—C11—C12—N6	0.0 (3)
C2—C1—C6—C5	−0.8 (3)	C13—N6—C12—C11	0.4 (3)
C7—C1—C6—C5	178.39 (19)	C12—N6—C13—N5	−0.6 (3)
N3—N2—C7—C1	102.0 (2)	C11—N5—C13—N6	0.7 (3)
C8—N2—C7—C1	−75.2 (3)	C10—N5—C13—N6	176.8 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.98 (2)	2.55 (2)	3.189 (2)	123.0 (18)
C7—H7*B*···N6^{ii}	0.95 (3)	2.60 (3)	3.478 (3)	154 (2)
C11—H11···O2^{iii}	0.98 (3)	2.66 (3)	3.535 (3)	149 (2)
C6—H6···N3^{iv}	1.00 (2)	2.54 (3)	3.299 (3)	133 (2)

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