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1-[(1-Butyl-1*H*-1,2,3-triazol-5-yl)methyl]-3-methylquinoxalin-2(1*H*)-one

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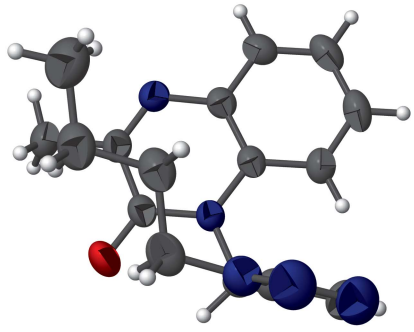
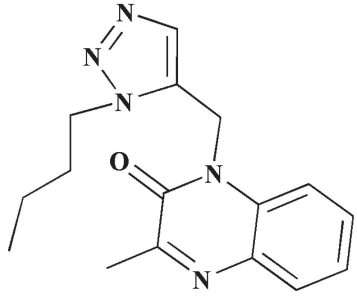
In the title compound, $C_{16}H_{19}N_5O$, the quinoxaline and triazole rings are almost orthogonal, inclined to one another at an angle of 79.8 (3)°. A weak intramolecular C—H···O interaction locks the conformation of the molecule. The crystal packing features weak intermolecular C—H···O and C—H···N interactions, which form chains along the *b*-axis direction. In addition, weak C—H···π intermolecular interactions further influence the crystal packing.

3D view



Chemical scheme



Structure description

The quinoxaline moiety is present in a variety of physiologically active compounds, with applications varying from medicinal to agricultural (Ramli *et al.*, 2014). Quinoxaline derivatives possess diverse biological activities showing insecticidal, fungicidal, herbicidal, anthelmintic and antiviral properties (Ramli & Essassi, 2015). As a continuation of our work on the synthesis of 3-methyl quinoxalin-2-one derivatives in order to evaluate their pharmacological activities (Ramli *et al.*, 2010*a*,*b*, 2011, 2013, 2017; Caleb *et al.*, 2016; Missioui *et al.*, 2017), the title compound (Fig. 1) was synthesized and its crystal structure is reported here. This compound is built up from the two fused six-membered rings of a quinoxalinone ring system linked through a methylene bridge to a 1,2,3-triazole ring, which in turn carries a *n*-butyl substituent on N3 (Sebbar *et al.*, 2016, Ellouz *et al.*, 2015).

The title compound crystallizes with one independent molecule in the asymmetric unit. The quinoxaline ring system is essentially planar with atom N4 showing a maximum deviation of 0.035 (9) Å from the mean plane of the ten-membered ring system. In addition, the quinoxaline ring system occupies an anti-clinal [C1—C2···C13—C14 =

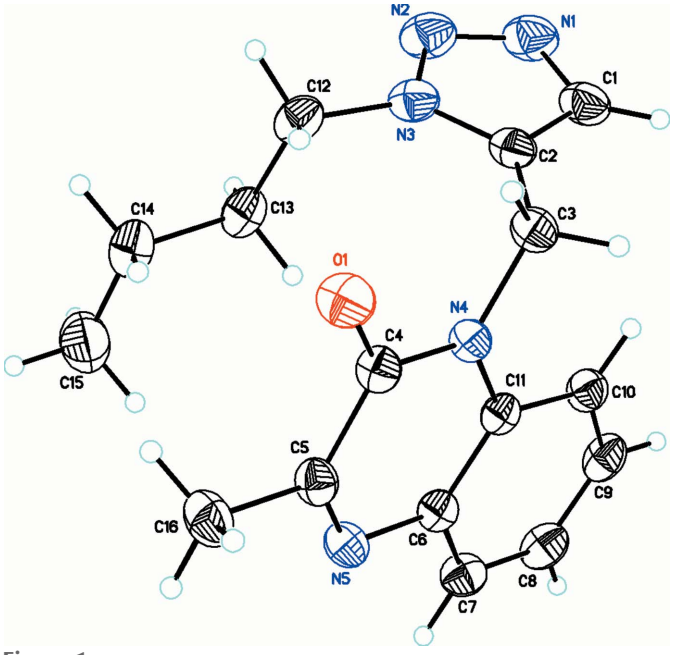


Figure 1
A view of the molecular structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level.

−119.8 (2)°] orientation with respect to the mean plane of the triazole ring and is twisted with a dihedral angle of 79.8 (3)° between this ring and the quinoxalinone ring system. The butyl moiety on the other hand is in a syn-clinal orientation [N2—N3—C12—C13 = 85.6 (2)] with respect to the triazole ring. A weak intramolecular C12—H12*B*···O1 interaction locks the conformation of the molecule (Fig. 2, Table 1).

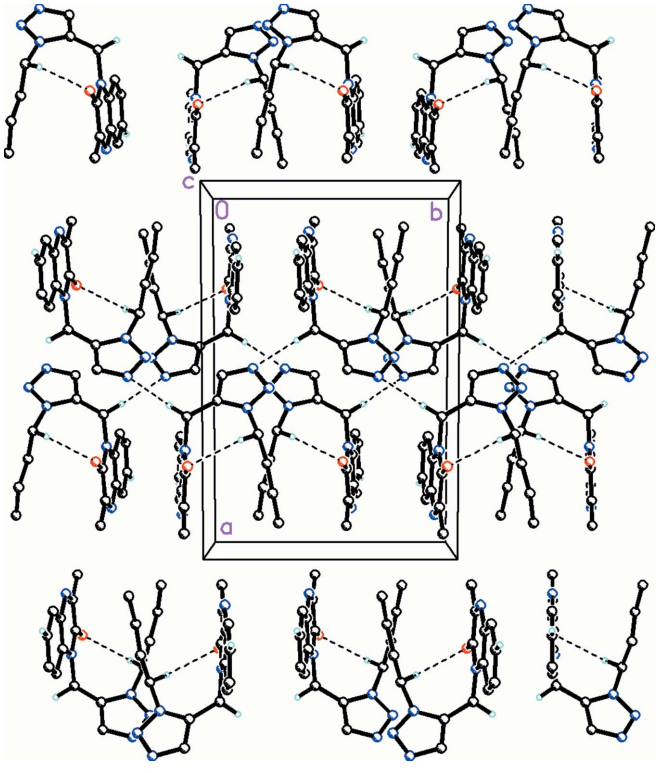


Figure 2
A partial view along the *c* axis of the crystal packing. Dashed lines indicate both weak C—H···O, C—H···N intermolecular and C—H···O intramolecular interactions. Atoms not involved in the hydrogen-bonding interactions have been omitted for clarity.

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the N1–N3/C1/C2, N4/N5/C4–C6/C11 and C6–C11 rings respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*B*···O1	0.97	2.48	3.335 (3)	147
C3—H3*A*···N1^{i}	0.97	2.45	3.416 (3)	176
C8—H8···O1^{ii}	0.93	2.58	3.251 (2)	130
C3—H3*B*···*Cg*1^{iii}	0.97	3.00	3.670 (2)	127
C13—H13*B*···*Cg*2	0.97	2.85	3.661 (2)	142
C14—H14*A*···*Cg*3^{iv}	0.97	2.84	3.724 (2)	152

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

The crystal packing features weak C—H···O and C—H···N intermolecular interactions forming chains along the *b*-axis direction (Fig. 2, Table 1). In addition, weak C3—H3*B*···π(*Cg*1), C13—H13*B*···π(*Cg*2) and C14—H14*A*···π(*Cg*3) intermolecular interactions, Table 1, further influence the crystal packing. No classical hydrogen bonds are observed.

Synthesis and crystallization

To a solution of 3-methyl-1-(prop-2-ynyl)-3,4-dihydroquinoxalin-2(1*H*)-one (0.68 mmol) in ethanol (15 ml) was

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{19}N_5O$
M_r	297.36
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, *b*, *c* (Å)	15.8299 (8), 10.6270 (4), 9.2041 (3)
β (°)	98.084 (4)
V (Å^3)	1532.97 (11)
Z	4
Radiation type	Cu *Kα*
μ (mm^{-1})	0.68
Crystal size (mm)	0.24 × 0.22 × 0.04
Data collection	
Diffractometer	Rigaku OD Xcalibur Eos Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.794, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5580, 2887, 2257
R_{int}	0.019
(sin θ/λ)$_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.053, 0.157, 1.02
No. of reflections	2887
No. of parameters	201
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.21

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

added 1-azidobutane (1.03 mmol). The reaction mixture was stirred under reflux for 72 h. After completion of the reaction (monitored by TLC), the solution was concentrated and the residue was purified by column chromatography on silica gel by using as eluent the mixture (hexane/ethyl acetate 8:2). The solid product obtained was crystallized from ethanol to afford colourless crystals in 16% yield.

Refinement

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

Funding information

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full crystallographic data

IUCrData (2018). **3**, x180482 [https://doi.org/10.1107/S2414314618004820]

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Crystal data

$C_{16}H_{19}N_5O$
M_r = 297.36
Monoclinic, $P2_1/c$
a = 15.8299 (8) Å
b = 10.6270 (4) Å
c = 9.2041 (3) Å
β = 98.084 (4)°
V = 1532.97 (11) Å^3
Z = 4
$F(000)$ = 632
D_x = 1.288 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 2219 reflections
θ = 5.0–71.3°
μ = 0.68 mm^{-1}
T = 293 K
Plate, colourless
0.24 × 0.22 × 0.04 mm

Data collection

Rigaku OD Xcalibur Eos Gemini diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.794, T_{max} = 1.000
5580 measured reflections
2887 independent reflections
2257 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 71.4°, θ_{min} = 5.0°
h = −19→18
k = −12→9
l = −11→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.157
S = 1.02
2887 reflections
201 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0798P)^2 + 0.4446P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.74544 (10)	0.55020 (16)	0.66870 (14)	0.0596 (4)
N1	0.48881 (13)	0.3093 (2)	0.2446 (2)	0.0697 (6)
N2	0.54195 (14)	0.2443 (2)	0.3387 (2)	0.0693 (6)
N3	0.59408 (11)	0.32718 (18)	0.41696 (19)	0.0546 (5)
N4	0.70864 (9)	0.57241 (14)	0.42118 (16)	0.0392 (4)
N5	0.88308 (10)	0.58729 (16)	0.39979 (17)	0.0463 (4)
C1	0.50794 (14)	0.4318 (2)	0.2624 (3)	0.0588 (6)
H1	0.479662	0.497079	0.208530	0.071*
C2	0.57542 (12)	0.4464 (2)	0.3720 (2)	0.0482 (5)
C3	0.61758 (12)	0.56295 (19)	0.4363 (2)	0.0470 (5)
H3A	0.588035	0.635325	0.389280	0.056*
H3B	0.611719	0.566253	0.539760	0.056*
C4	0.76751 (12)	0.56566 (18)	0.54693 (19)	0.0424 (4)
C5	0.85801 (12)	0.57422 (18)	0.5260 (2)	0.0440 (4)
C6	0.82194 (12)	0.59686 (17)	0.27565 (19)	0.0410 (4)
C7	0.85021 (14)	0.6119 (2)	0.1395 (2)	0.0510 (5)
H7	0.908390	0.615156	0.134056	0.061*
C8	0.79259 (16)	0.6219 (2)	0.0140 (2)	0.0562 (5)
H8	0.811729	0.630647	−0.076527	0.067*
C9	0.70609 (15)	0.6191 (2)	0.0220 (2)	0.0550 (5)
H9	0.667359	0.626632	−0.063395	0.066*
C10	0.67642 (13)	0.60513 (19)	0.1549 (2)	0.0468 (5)
H10	0.618071	0.604692	0.159195	0.056*
C11	0.73449 (12)	0.59165 (16)	0.28335 (19)	0.0385 (4)
C12	0.66329 (15)	0.2808 (2)	0.5264 (2)	0.0588 (6)
H12A	0.644317	0.205872	0.572596	0.071*
H12B	0.676992	0.344162	0.601957	0.071*
C13	0.74284 (15)	0.2501 (2)	0.4584 (2)	0.0566 (5)
H13A	0.731888	0.176846	0.395742	0.068*
H13B	0.755878	0.320089	0.397712	0.068*
C14	0.81893 (16)	0.2243 (2)	0.5732 (3)	0.0644 (6)
H14A	0.807379	0.150401	0.629041	0.077*
H14B	0.826964	0.294931	0.640492	0.077*
C15	0.90023 (18)	0.2033 (3)	0.5077 (3)	0.0875 (9)
H15A	0.911247	0.275242	0.450146	0.131*
H15B	0.894122	0.129902	0.446367	0.131*
H15C	0.946930	0.191470	0.585121	0.131*
C16	0.92225 (14)	0.5652 (2)	0.6610 (2)	0.0594 (6)
H16A	0.912318	0.489923	0.713739	0.089*
H16B	0.917122	0.637133	0.722238	0.089*
H16C	0.978585	0.562721	0.633781	0.089*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0602 (9)	0.0843 (11)	0.0344 (7)	−0.0058 (8)	0.0071 (6)	−0.0005 (7)
N1	0.0594 (11)	0.0780 (14)	0.0691 (12)	−0.0220 (11)	−0.0001 (9)	−0.0034 (11)
N2	0.0713 (13)	0.0620 (12)	0.0736 (13)	−0.0227 (10)	0.0067 (10)	−0.0045 (10)
N3	0.0539 (10)	0.0579 (10)	0.0521 (10)	−0.0120 (8)	0.0080 (8)	−0.0005 (8)
N4	0.0398 (8)	0.0417 (8)	0.0353 (7)	−0.0011 (6)	0.0023 (6)	−0.0029 (6)
N5	0.0421 (8)	0.0525 (9)	0.0439 (9)	0.0014 (7)	0.0046 (7)	−0.0046 (7)
C1	0.0438 (10)	0.0697 (14)	0.0614 (13)	−0.0123 (10)	0.0018 (9)	−0.0015 (11)
C2	0.0405 (9)	0.0574 (12)	0.0480 (10)	−0.0045 (9)	0.0103 (8)	0.0004 (9)
C3	0.0435 (10)	0.0525 (11)	0.0455 (10)	−0.0004 (9)	0.0078 (8)	−0.0040 (8)
C4	0.0471 (10)	0.0445 (10)	0.0347 (9)	−0.0004 (8)	0.0022 (7)	−0.0034 (7)
C5	0.0449 (10)	0.0443 (10)	0.0409 (9)	0.0020 (8)	−0.0005 (8)	−0.0039 (8)
C6	0.0464 (10)	0.0381 (9)	0.0382 (9)	−0.0005 (8)	0.0049 (7)	−0.0032 (7)
C7	0.0557 (11)	0.0526 (11)	0.0472 (10)	−0.0012 (9)	0.0157 (9)	−0.0019 (9)
C8	0.0788 (15)	0.0545 (12)	0.0367 (9)	−0.0053 (11)	0.0124 (9)	0.0018 (9)
C9	0.0744 (14)	0.0495 (11)	0.0372 (9)	−0.0046 (10)	−0.0060 (9)	0.0050 (8)
C10	0.0482 (10)	0.0472 (10)	0.0429 (10)	−0.0026 (8)	−0.0012 (8)	0.0029 (8)
C11	0.0469 (10)	0.0334 (8)	0.0346 (8)	−0.0007 (7)	0.0033 (7)	−0.0015 (6)
C12	0.0709 (14)	0.0569 (12)	0.0488 (11)	−0.0055 (11)	0.0087 (10)	0.0092 (9)
C13	0.0723 (14)	0.0498 (11)	0.0465 (11)	0.0008 (10)	0.0039 (10)	0.0035 (9)
C14	0.0789 (16)	0.0565 (13)	0.0548 (12)	0.0086 (11)	−0.0009 (11)	0.0046 (10)
C15	0.0768 (18)	0.096 (2)	0.0858 (19)	0.0122 (16)	−0.0010 (15)	0.0102 (17)
C16	0.0489 (11)	0.0771 (15)	0.0488 (11)	0.0032 (11)	−0.0049 (9)	−0.0002 (10)

Geometric parameters (Å, º)

O1—C4	1.231 (2)	C8—H8	0.9300
N1—N2	1.316 (3)	C8—C9	1.382 (3)
N1—C1	1.342 (3)	C9—H9	0.9300
N2—N3	1.345 (3)	C9—C10	1.379 (3)
N3—C2	1.353 (3)	C10—H10	0.9300
N3—C12	1.466 (3)	C10—C11	1.399 (3)
N4—C3	1.471 (2)	C12—H12A	0.9700
N4—C4	1.382 (2)	C12—H12B	0.9700
N4—C11	1.402 (2)	C12—C13	1.518 (3)
N5—C5	1.287 (2)	C13—H13A	0.9700
N5—C6	1.393 (2)	C13—H13B	0.9700
C1—H1	0.9300	C13—C14	1.511 (3)
C1—C2	1.371 (3)	C14—H14A	0.9700
C2—C3	1.489 (3)	C14—H14B	0.9700
C3—H3A	0.9700	C14—C15	1.512 (4)
C3—H3B	0.9700	C15—H15A	0.9600
C4—C5	1.475 (3)	C15—H15B	0.9600
C5—C16	1.494 (3)	C15—H15C	0.9600
C6—C7	1.397 (3)	C16—H16A	0.9600
C6—C11	1.397 (3)	C16—H16B	0.9600

C7—H7	0.9300	C16—H16C	0.9600
C7—C8	1.372 (3)		

N2—N1—C1	108.45 (19)	C10—C9—H9	119.5
N1—N2—N3	107.2 (2)	C9—C10—H10	120.2
N2—N3—C2	111.02 (19)	C9—C10—C11	119.69 (19)
N2—N3—C12	119.4 (2)	C11—C10—H10	120.2
C2—N3—C12	129.44 (19)	C6—C11—N4	117.98 (15)
C4—N4—C3	118.12 (15)	C6—C11—C10	119.42 (17)
C4—N4—C11	121.15 (15)	C10—C11—N4	122.60 (17)
C11—N4—C3	120.70 (15)	N3—C12—H12A	109.2
C5—N5—C6	118.76 (16)	N3—C12—H12B	109.2
N1—C1—H1	125.1	N3—C12—C13	111.84 (17)
N1—C1—C2	109.8 (2)	H12A—C12—H12B	107.9
C2—C1—H1	125.1	C13—C12—H12A	109.2
N3—C2—C1	103.48 (19)	C13—C12—H12B	109.2
N3—C2—C3	126.22 (18)	C12—C13—H13A	109.2
C1—C2—C3	130.2 (2)	C12—C13—H13B	109.2
N4—C3—C2	114.17 (15)	H13A—C13—H13B	107.9
N4—C3—H3A	108.7	C14—C13—C12	112.13 (18)
N4—C3—H3B	108.7	C14—C13—H13A	109.2
C2—C3—H3A	108.7	C14—C13—H13B	109.2
C2—C3—H3B	108.7	C13—C14—H14A	109.0
H3A—C3—H3B	107.6	C13—C14—H14B	109.0
O1—C4—N4	121.69 (17)	C13—C14—C15	112.8 (2)
O1—C4—C5	122.16 (17)	H14A—C14—H14B	107.8
N4—C4—C5	116.12 (15)	C15—C14—H14A	109.0
N5—C5—C4	123.58 (16)	C15—C14—H14B	109.0
N5—C5—C16	119.83 (18)	C14—C15—H15A	109.5
C4—C5—C16	116.58 (17)	C14—C15—H15B	109.5
N5—C6—C7	118.05 (17)	C14—C15—H15C	109.5
N5—C6—C11	122.31 (16)	H15A—C15—H15B	109.5
C11—C6—C7	119.64 (17)	H15A—C15—H15C	109.5
C6—C7—H7	119.8	H15B—C15—H15C	109.5
C8—C7—C6	120.3 (2)	C5—C16—H16A	109.5
C8—C7—H7	119.8	C5—C16—H16B	109.5
C7—C8—H8	120.0	C5—C16—H16C	109.5
C7—C8—C9	119.95 (18)	H16A—C16—H16B	109.5
C9—C8—H8	120.0	H16A—C16—H16C	109.5
C8—C9—H9	119.5	H16B—C16—H16C	109.5
C10—C9—C8	120.92 (19)		

O1—C4—C5—N5	178.3 (2)	C3—N4—C11—C10	1.2 (3)
O1—C4—C5—C16	−0.9 (3)	C4—N4—C3—C2	−112.54 (19)
N1—N2—N3—C2	−0.8 (2)	C4—N4—C11—C6	3.5 (2)
N1—N2—N3—C12	−176.99 (18)	C4—N4—C11—C10	−176.77 (17)
N1—C1—C2—N3	−0.3 (2)	C5—N5—C6—C7	179.55 (18)
N1—C1—C2—C3	−177.2 (2)	C5—N5—C6—C11	−0.6 (3)

N2—N1—C1—C2	−0.2 (3)	C6—N5—C5—C4	1.5 (3)
N2—N3—C2—C1	0.7 (2)	C6—N5—C5—C16	−179.32 (18)
N2—N3—C2—C3	177.76 (18)	C6—C7—C8—C9	1.0 (3)
N2—N3—C12—C13	85.6 (2)	C7—C6—C11—N4	177.98 (17)
N3—C2—C3—N4	63.9 (3)	C7—C6—C11—C10	−1.8 (3)
N3—C12—C13—C14	169.95 (19)	C7—C8—C9—C10	−0.6 (3)
N4—C4—C5—N5	0.0 (3)	C8—C9—C10—C11	−1.0 (3)
N4—C4—C5—C16	−179.16 (18)	C9—C10—C11—N4	−177.55 (17)
N5—C6—C7—C8	−179.93 (19)	C9—C10—C11—C6	2.2 (3)
N5—C6—C11—N4	−1.9 (3)	C11—N4—C3—C2	69.4 (2)
N5—C6—C11—C10	178.35 (17)	C11—N4—C4—O1	179.18 (17)
C1—N1—N2—N3	0.6 (3)	C11—N4—C4—C5	−2.6 (2)
C1—C2—C3—N4	−119.8 (2)	C11—C6—C7—C8	0.2 (3)
C2—N3—C12—C13	−89.8 (3)	C12—N3—C2—C1	176.3 (2)
C3—N4—C4—O1	1.1 (3)	C12—N3—C2—C3	−6.6 (3)
C3—N4—C4—C5	179.36 (15)	C12—C13—C14—C15	−175.6 (2)
C3—N4—C11—C6	−178.52 (15)		

Hydrogen-bond geometry (Å, º)

Cg1, Cg2 and Cg3 are the centroids of the N1–N3/C1/C2, N4/N5/C4–C6/C11 and C6–C11 rings respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*B*···O1	0.97	2.48	3.335 (3)	147
C3—H3*A*···N1^{i}	0.97	2.45	3.416 (3)	176
C8—H8···O1^{ii}	0.93	2.58	3.251 (2)	130
C3—H3*B*···*Cg*1^{iii}	0.97	3.00	3.670 (2)	127
C13—H13*B*···*Cg*2	0.97	2.85	3.661 (2)	142
C14—H14*A*···*Cg*3^{iv}	0.97	2.84	3.724 (2)	152

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