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Diethyl 1-[(4-methyl-2-phenyl-4,5-dihydro-1,3-oxazol-4-yl)methyl]-1*H*-1,2,3-triazole-4,5-dicarboxylate

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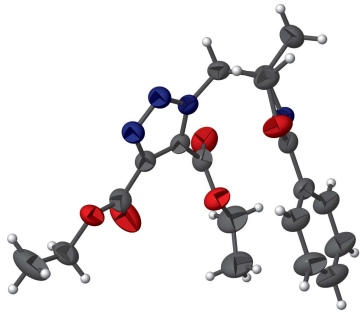
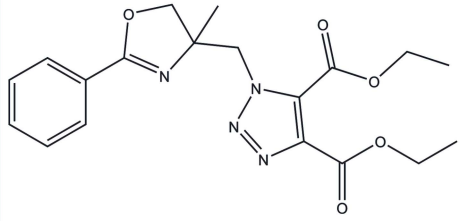
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{19}H_{22}N_4O_5$, the central triazole ring makes dihedral angles of 56.15 (8) and 43.25 (9)° with the oxazole and benzene rings, respectively. The mean planes of the two ethoxycarbonyl groups make dihedral angles of 24.16 (11) and 51.90 (10)° with the triazole ring. Globally, the molecule has a U-shape. In the crystal, molecules are linked by C—H···O and C—H···N hydrogen bonds into supramolecular layers in the *bc* plane.

3D view



Chemical scheme



Structure description

Azide–alkyne cycloaddition is a useful and convenient method for the preparation of 1,2,3-triazoles (Lutz *et al.*, 2008; Oliva *et al.*, 2008; Kiss *et al.*, 2010). The approach for the synthesis of 1,2,3-triazole-substituted compounds involves transformation of the azide function in a 1,3-dipolar cycloaddition reaction with acetylene derivatives. In this context, the title compound was obtained with good yield (Boukhssas *et al.*, 2017).

In the title compound, Fig. 1, the central triazole ring is planar (r.m.s deviation = 0.0054 (13) Å) and makes dihedral angles of 56.15 (8) and 43.25 (9)° with the oxazol and benzene rings, respectively. The mean planes of the two ethoxycarbonyl groups make dihedral angles of 24.16 (11) and 51.90 (10)° with the triazole ring.

In the crystal, molecules are linked by C—H···O and C—H···N hydrogen bonds into supramolecular layers in the *bc* plane, Table 1 and Fig. 2.

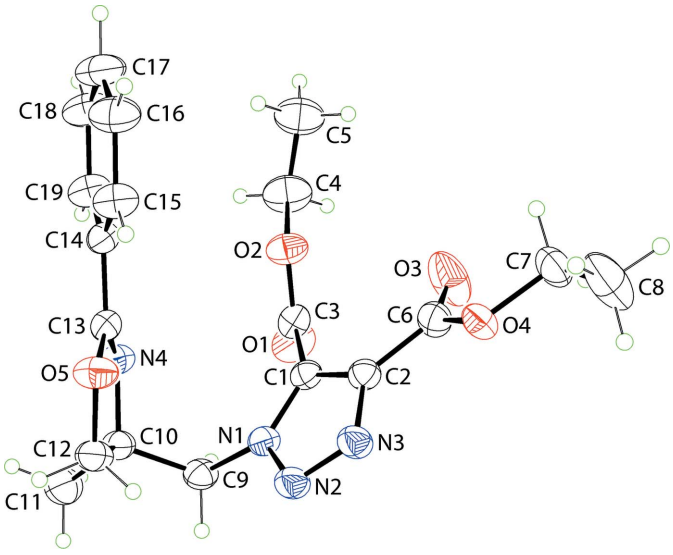


Figure 1
The structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level. H atoms are represented as small spheres of arbitrary radii.

Synthesis and crystallization

A mixture of 4-(azidomethyl)-4-methyl-2-phenyl-4,5-dihydrooxazole (0.65 mmol) and diethyl acetylenedicarboxylate (0.65 mmol) was stirred for 12 h. The crude product was treated with ethyl acetate, the organic layer was washed with water, dried with Na_2SO_4, and the solvent removed. The product was purified by recrystallization from ether–hexane to afford the pure product. Suitable crystals of the title compound were obtained by recrystallization from its $CHCl_3$ solution. The structure of the product was established on the basis of NMR spectroscopy (^{1}H and ^{13}C) and MS data.

Yield = 75% (white solid); m.p. = 92–94°C; R_f = 0.23 (ether/hexane). ^{1}H NMR (300.13 MHz; $CDCl_3$): 1.30 (3*H*, **CH$_3$**–CH$_2$, *t*, *J* = 7.15 Hz); 1.38 (3*H*, **CH$_3$**–CH$_2$, *t*, *J* = 7.14 Hz); 1.41 (3*H*, **CH$_3$**–Oxaz, s); 4.13–4.53 (2*H*, **CH$_2$**–Oxaz, *AB*, *J* = 9.05 Hz); 4.24–4.38 (2*H*, –**CH$_2$**–CH$_3$, *q*, *J* = 7.15 Hz); 4.27–4.42 (2*H*, –**CH$_2$**–CH$_3$, *q*, *J* = 7.15 Hz); 4.76–4.93 (2*H*, --**CH$_2$**–triazole, *AB*, *J* = 13.76 Hz); 7.35–7.84 (5Harom, *m*). ^{13}C NMR (75.47 MHz; $CDCl_3$): 13.66 (**C**H$_3$–CH$_2$); 14.14 (**C**H$_3$–CH$_2$); 25.22 (**C**H$_3$–Oxaz); 56.38 (**C**H$_2$–triazole); 61.71 (CH$_3$–**C**H$_2$); 62.76 (CH$_3$–**C**H$_2$); 70.77 (**C$_q$**–Oxaz); 75.13 (**C**H$_2$–Oxaz); 127.00 (**C**-5, of triazole ring); 128.21; 128.46; 131.74 and 132.06 (6 **C**arom); 139.60 (**C**-4, of triazole ring); 158.73 and 159.93 (**C**O); 164.46 (**C**N). MS–EI: $[M+1]^+$= 387.

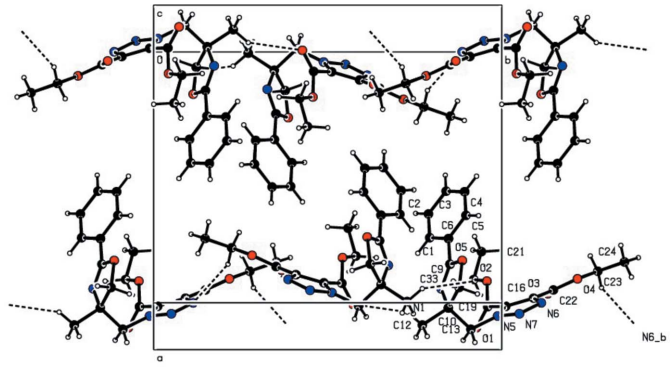


Figure 2
A view of the molecular packing along the *c* axis. Hydrogen bonds are drawn as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*B*···N3^{i}	0.97	2.59	3.454 (2)	149
C11—H11*A*···O1^{ii}	0.96	2.56	3.392 (2)	145

Symmetry codes: (i) $x, -y+\frac{5}{2}, z-\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{22}N_4O_5$
M_r	386.41
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, *b*, *c* (Å)	13.9450 (9), 16.3245 (10), 9.0473 (6)
β (°)	104.066 (2)
V (Å^3)	1997.8 (2)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.10
Crystal size (mm)	0.34 × 0.21 × 0.17
Data collection	
Diffractometer	Bruker APEXII CCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33174, 3529, 2938
R_{int}	0.032
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.037, 0.108, 1.07
No. of reflections	3529
No. of parameters	257
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.26

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS2013* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

Refinement

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

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full crystallographic data

IUCrData (2017). **2**, x171701 [https://doi.org/10.1107/S2414314617017011]

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Crystal data

$C_{19}H_{22}N_4O_5$
M_r = 386.41
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 13.9450 (9) Å
b = 16.3245 (10) Å
c = 9.0473 (6) Å
β = 104.066 (2)°
V = 1997.8 (2) Å^3
Z = 4
$F(000)$ = 816
D_x = 1.285 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 298 reflections
θ = 1.4–28.4°
μ = 0.10 mm^{-1}
T = 173 K
Prism, colourless
0.34 × 0.21 × 0.17 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
33174 measured reflections
3529 independent reflections
2938 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 25.0°, θ_{min} = 2.5°
h = −16→16
k = −19→19
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.108
S = 1.07
3529 reflections
257 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2 + 0.3505P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0066 (12)

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	0.91074 (9)	0.92709 (7)	−0.10242 (14)	0.0694 (4)
O2	0.75141 (8)	0.95729 (7)	−0.11812 (12)	0.0566 (3)
O3	0.78857 (14)	1.13220 (8)	−0.14989 (14)	0.0965 (5)
O4	0.76719 (8)	1.21752 (6)	0.03184 (11)	0.0509 (3)
O5	0.75886 (7)	0.88651 (7)	0.37008 (12)	0.0594 (3)
N1	0.92249 (8)	0.98814 (7)	0.22234 (13)	0.0422 (3)
N2	0.93045 (9)	1.05074 (7)	0.32281 (14)	0.0503 (3)
N3	0.88258 (9)	1.11341 (7)	0.25090 (13)	0.0485 (3)
N4	0.82672 (9)	0.82643 (7)	0.19534 (14)	0.0495 (3)
C1	0.86797 (9)	1.01117 (8)	0.08517 (15)	0.0401 (3)
C2	0.84362 (10)	1.09149 (8)	0.10399 (15)	0.0421 (3)
C3	0.84737 (11)	0.95944 (9)	−0.05463 (16)	0.0465 (3)
C4	0.72235 (16)	0.91941 (14)	−0.2678 (2)	0.0810 (6)
H4A	0.7292	0.8604	−0.2587	0.097*
H4B	0.7642	0.9389	−0.3317	0.097*
C5	0.61798 (18)	0.94152 (15)	−0.3363 (2)	0.0955 (7)
H5A	0.5771	0.9219	−0.2723	0.143*
H5B	0.5971	0.9170	−0.4353	0.143*
H5C	0.6121	1.0000	−0.3455	0.143*
C6	0.79680 (12)	1.14840 (9)	−0.01821 (16)	0.0506 (4)
C7	0.72300 (14)	1.27614 (10)	−0.08724 (19)	0.0635 (4)
H7A	0.6618	1.2543	−0.1497	0.076*
H7B	0.7678	1.2865	−0.1522	0.076*
C8	0.7035 (2)	1.35238 (13)	−0.0141 (2)	0.1027 (8)
H8A	0.6570	1.3421	0.0463	0.154*
H8B	0.6768	1.3924	−0.0909	0.154*
H8C	0.7641	1.3726	0.0500	0.154*
C9	0.97441 (10)	0.91127 (9)	0.27105 (18)	0.0484 (4)
H9A	1.0317	0.9228	0.3536	0.058*
H9B	0.9981	0.8892	0.1869	0.058*
C10	0.91134 (10)	0.84644 (8)	0.32417 (17)	0.0480 (4)
C11	0.97659 (14)	0.77174 (10)	0.3755 (2)	0.0743 (5)
H11A	0.9375	0.7284	0.4023	0.111*
H11B	1.0286	0.7859	0.4625	0.111*
H11C	1.0047	0.7539	0.2941	0.111*
C12	0.86204 (11)	0.87770 (11)	0.44759 (17)	0.0558 (4)
H12A	0.8702	0.8387	0.5306	0.067*
H12B	0.8900	0.9299	0.4880	0.067*
C13	0.74973 (10)	0.85130 (8)	0.23094 (16)	0.0448 (3)

C14	0.64819 (10)	0.84697 (9)	0.13450 (17)	0.0477 (4)
C15	0.57447 (12)	0.89708 (11)	0.1616 (2)	0.0630 (4)
H15	0.5883	0.9334	0.2433	0.076*
C16	0.48023 (13)	0.89344 (14)	0.0675 (2)	0.0753 (5)
H16	0.4309	0.9275	0.0857	0.090*
C17	0.45948 (13)	0.83999 (14)	−0.0518 (2)	0.0778 (6)
H17	0.3961	0.8378	−0.1152	0.093*
C18	0.53193 (14)	0.78945 (14)	−0.0784 (2)	0.0795 (6)
H18	0.5172	0.7526	−0.1591	0.095*
C19	0.62626 (13)	0.79287 (11)	0.0134 (2)	0.0630 (4)
H19	0.6753	0.7588	−0.0061	0.076*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0646 (7)	0.0756 (8)	0.0763 (8)	−0.0012 (6)	0.0331 (6)	−0.0257 (6)
O2	0.0532 (6)	0.0723 (7)	0.0424 (6)	−0.0056 (5)	0.0080 (5)	−0.0191 (5)
O3	0.1746 (16)	0.0726 (8)	0.0387 (7)	0.0207 (9)	0.0192 (8)	0.0032 (6)
O4	0.0572 (6)	0.0520 (6)	0.0406 (6)	0.0088 (5)	0.0060 (5)	0.0069 (4)
O5	0.0456 (6)	0.0838 (8)	0.0460 (6)	−0.0019 (5)	0.0058 (5)	−0.0103 (5)
N1	0.0384 (6)	0.0426 (6)	0.0439 (6)	−0.0020 (5)	0.0067 (5)	−0.0030 (5)
N2	0.0558 (7)	0.0458 (7)	0.0431 (7)	−0.0008 (6)	−0.0001 (6)	−0.0041 (5)
N3	0.0561 (7)	0.0454 (6)	0.0396 (7)	0.0007 (5)	0.0031 (5)	−0.0038 (5)
N4	0.0424 (7)	0.0503 (7)	0.0520 (7)	−0.0029 (5)	0.0040 (6)	−0.0057 (5)
C1	0.0364 (7)	0.0449 (7)	0.0399 (7)	−0.0048 (6)	0.0110 (6)	−0.0033 (6)
C2	0.0433 (7)	0.0457 (7)	0.0370 (7)	−0.0035 (6)	0.0093 (6)	−0.0027 (6)
C3	0.0515 (9)	0.0460 (7)	0.0458 (8)	−0.0048 (6)	0.0189 (7)	−0.0065 (6)
C4	0.0879 (14)	0.0981 (14)	0.0515 (10)	−0.0074 (11)	0.0062 (10)	−0.0337 (10)
C5	0.0958 (16)	0.1154 (18)	0.0590 (12)	−0.0133 (13)	−0.0128 (11)	−0.0138 (11)
C6	0.0610 (9)	0.0516 (8)	0.0389 (8)	−0.0037 (7)	0.0114 (7)	0.0004 (6)
C7	0.0762 (11)	0.0596 (10)	0.0493 (9)	0.0064 (8)	0.0048 (8)	0.0160 (7)
C8	0.159 (2)	0.0744 (13)	0.0639 (12)	0.0469 (14)	0.0051 (14)	0.0081 (10)
C9	0.0365 (7)	0.0488 (8)	0.0574 (9)	0.0061 (6)	0.0064 (6)	−0.0003 (7)
C10	0.0415 (8)	0.0449 (7)	0.0518 (9)	−0.0004 (6)	0.0002 (6)	−0.0002 (6)
C11	0.0688 (11)	0.0511 (9)	0.0917 (14)	0.0070 (8)	−0.0024 (10)	0.0086 (9)
C12	0.0470 (8)	0.0709 (10)	0.0446 (8)	−0.0075 (7)	0.0018 (7)	0.0023 (7)
C13	0.0461 (8)	0.0425 (7)	0.0440 (8)	−0.0071 (6)	0.0077 (6)	0.0008 (6)
C14	0.0416 (8)	0.0529 (8)	0.0474 (8)	−0.0087 (6)	0.0084 (6)	0.0021 (7)
C15	0.0499 (9)	0.0755 (11)	0.0604 (10)	−0.0015 (8)	0.0073 (8)	−0.0110 (8)
C16	0.0457 (9)	0.1039 (14)	0.0738 (12)	0.0070 (9)	0.0100 (9)	−0.0087 (11)
C17	0.0439 (9)	0.1183 (16)	0.0649 (12)	−0.0127 (10)	0.0011 (8)	−0.0090 (11)
C18	0.0589 (11)	0.1041 (15)	0.0685 (12)	−0.0138 (10)	0.0020 (9)	−0.0284 (11)
C19	0.0492 (9)	0.0733 (11)	0.0633 (10)	−0.0064 (8)	0.0075 (8)	−0.0149 (8)

Geometric parameters (Å, º)

O1—C3	1.1969 (17)	C7—H7B	0.9700
O2—C3	1.3222 (18)	C8—H8A	0.9600

O2—C4	1.4543 (19)	C8—H8B	0.9600
O3—C6	1.1983 (18)	C8—H8C	0.9600
O4—C6	1.3190 (18)	C9—C10	1.526 (2)
O4—C7	1.4606 (18)	C9—H9A	0.9700
O5—C13	1.3614 (17)	C9—H9B	0.9700
O5—C12	1.4464 (18)	C10—C11	1.525 (2)
N1—C1	1.3419 (17)	C10—C12	1.534 (2)
N1—N2	1.3542 (16)	C11—H11A	0.9600
N1—C9	1.4622 (18)	C11—H11B	0.9600
N2—N3	1.3055 (16)	C11—H11C	0.9600
N3—C2	1.3561 (17)	C12—H12A	0.9700
N4—C13	1.2607 (18)	C12—H12B	0.9700
N4—C10	1.4795 (19)	C13—C14	1.473 (2)
C1—C2	1.3753 (19)	C14—C15	1.382 (2)
C1—C3	1.4896 (19)	C14—C19	1.383 (2)
C2—C6	1.470 (2)	C15—C16	1.383 (2)
C4—C5	1.481 (3)	C15—H15	0.9300
C4—H4A	0.9700	C16—C17	1.364 (3)
C4—H4B	0.9700	C16—H16	0.9300
C5—H5A	0.9600	C17—C18	1.370 (3)
C5—H5B	0.9600	C17—H17	0.9300
C5—H5C	0.9600	C18—C19	1.376 (3)
C7—C8	1.465 (3)	C18—H18	0.9300
C7—H7A	0.9700	C19—H19	0.9300

C3—O2—C4	116.06 (12)	N1—C9—C10	114.14 (11)
C6—O4—C7	114.73 (12)	N1—C9—H9A	108.7
C13—O5—C12	105.35 (11)	C10—C9—H9A	108.7
C1—N1—N2	110.18 (11)	N1—C9—H9B	108.7
C1—N1—C9	130.31 (12)	C10—C9—H9B	108.7
N2—N1—C9	119.44 (11)	H9A—C9—H9B	107.6
N3—N2—N1	107.95 (11)	N4—C10—C11	111.47 (12)
N2—N3—C2	108.44 (11)	N4—C10—C9	108.38 (12)
C13—N4—C10	107.05 (12)	C11—C10—C9	107.67 (13)
N1—C1—C2	104.72 (11)	N4—C10—C12	103.54 (11)
N1—C1—C3	125.13 (12)	C11—C10—C12	112.58 (14)
C2—C1—C3	130.02 (13)	C9—C10—C12	113.14 (12)
N3—C2—C1	108.70 (12)	C10—C11—H11A	109.5
N3—C2—C6	124.71 (12)	C10—C11—H11B	109.5
C1—C2—C6	125.97 (12)	H11A—C11—H11B	109.5
O1—C3—O2	126.13 (14)	C10—C11—H11C	109.5
O1—C3—C1	123.36 (14)	H11A—C11—H11C	109.5
O2—C3—C1	110.48 (11)	H11B—C11—H11C	109.5
O2—C4—C5	107.98 (16)	O5—C12—C10	104.43 (11)
O2—C4—H4A	110.1	O5—C12—H12A	110.9
C5—C4—H4A	110.1	C10—C12—H12A	110.9
O2—C4—H4B	110.1	O5—C12—H12B	110.9
C5—C4—H4B	110.1	C10—C12—H12B	110.9

H4A—C4—H4B	108.4	H12A—C12—H12B	108.9
C4—C5—H5A	109.5	N4—C13—O5	118.56 (13)
C4—C5—H5B	109.5	N4—C13—C14	126.07 (13)
H5A—C5—H5B	109.5	O5—C13—C14	115.36 (12)
C4—C5—H5C	109.5	C15—C14—C19	119.22 (15)
H5A—C5—H5C	109.5	C15—C14—C13	121.06 (14)
H5B—C5—H5C	109.5	C19—C14—C13	119.71 (14)
O3—C6—O4	124.59 (14)	C14—C15—C16	120.15 (16)
O3—C6—C2	121.74 (14)	C14—C15—H15	119.9
O4—C6—C2	113.66 (12)	C16—C15—H15	119.9
O4—C7—C8	108.35 (14)	C17—C16—C15	120.13 (18)
O4—C7—H7A	110.0	C17—C16—H16	119.9
C8—C7—H7A	110.0	C15—C16—H16	119.9
O4—C7—H7B	110.0	C16—C17—C18	120.06 (17)
C8—C7—H7B	110.0	C16—C17—H17	120.0
H7A—C7—H7B	108.4	C18—C17—H17	120.0
C7—C8—H8A	109.5	C17—C18—C19	120.48 (18)
C7—C8—H8B	109.5	C17—C18—H18	119.8
H8A—C8—H8B	109.5	C19—C18—H18	119.8
C7—C8—H8C	109.5	C18—C19—C14	119.95 (17)
H8A—C8—H8C	109.5	C18—C19—H19	120.0
H8B—C8—H8C	109.5	C14—C19—H19	120.0

C1—N1—N2—N3	−0.62 (15)	N2—N1—C9—C10	95.08 (15)
C9—N1—N2—N3	176.55 (11)	C13—N4—C10—C11	128.55 (15)
N1—N2—N3—C2	−0.01 (15)	C13—N4—C10—C9	−113.13 (13)
N2—N1—C1—C2	0.96 (14)	C13—N4—C10—C12	7.27 (15)
C9—N1—C1—C2	−175.80 (12)	N1—C9—C10—N4	61.10 (16)
N2—N1—C1—C3	177.17 (12)	N1—C9—C10—C11	−178.19 (13)
C9—N1—C1—C3	0.4 (2)	N1—C9—C10—C12	−53.13 (16)
N2—N3—C2—C1	0.61 (16)	C13—O5—C12—C10	9.24 (15)
N2—N3—C2—C6	−170.79 (13)	N4—C10—C12—O5	−10.01 (15)
N1—C1—C2—N3	−0.96 (15)	C11—C10—C12—O5	−130.54 (13)
C3—C1—C2—N3	−176.90 (13)	C9—C10—C12—O5	107.10 (13)
N1—C1—C2—C6	170.31 (13)	C10—N4—C13—O5	−1.56 (17)
C3—C1—C2—C6	−5.6 (2)	C10—N4—C13—C14	177.70 (13)
C4—O2—C3—O1	−7.0 (2)	C12—O5—C13—N4	−5.31 (17)
C4—O2—C3—C1	170.88 (14)	C12—O5—C13—C14	175.35 (12)
N1—C1—C3—O1	−53.3 (2)	N4—C13—C14—C15	−159.58 (16)
C2—C1—C3—O1	121.89 (18)	O5—C13—C14—C15	19.7 (2)
N1—C1—C3—O2	128.71 (14)	N4—C13—C14—C19	19.4 (2)
C2—C1—C3—O2	−56.09 (19)	O5—C13—C14—C19	−161.28 (14)
C3—O2—C4—C5	−165.55 (16)	C19—C14—C15—C16	−0.6 (3)
C7—O4—C6—O3	−0.8 (2)	C13—C14—C15—C16	178.45 (16)
C7—O4—C6—C2	178.29 (13)	C14—C15—C16—C17	0.4 (3)
N3—C2—C6—O3	158.83 (17)	C15—C16—C17—C18	0.3 (3)
C1—C2—C6—O3	−11.1 (2)	C16—C17—C18—C19	−0.9 (3)
N3—C2—C6—O4	−20.2 (2)	C17—C18—C19—C14	0.7 (3)

C1—C2—C6—O4	169.83 (13)	C15—C14—C19—C18	0.0 (3)
C6—O4—C7—C8	−174.17 (17)	C13—C14—C19—C18	−179.03 (17)
C1—N1—C9—C10	−88.40 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*B*···N3^{i}	0.97	2.59	3.454 (2)	149
C11—H11*A*···O1^{ii}	0.96	2.56	3.392 (2)	145

Symmetry codes: (i) *x*, −*y*+5/2, *z*−1/2; (ii) *x*, −*y*+3/2, *z*+1/2.