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1-(4-Nitrophenoxymethyl)-1*H*-1,2,4-triazole

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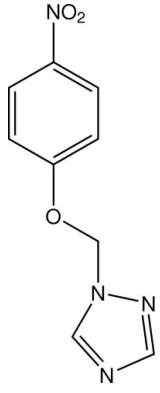
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.053; wR factor = 0.134; data-to-parameter ratio = 13.3.

The asymmetric unit of the title compound, $C_9H_8N_4O_3$, contains two independent molecules. The dihedral angles formed by the triazole and benzene rings in the two independent molecules are 83.3 (3) and 86.9 (4)°. The molecular packing involves weak C—H···N and C—H···O interactions, and π–π stacking interactions [centroid-to-centroid distance 3.745 (1) Å] between the aromatic rings of pairs of molecules.

Related literature

For the synthesis of related energetic polynitro and heterocyclic compounds, see: Jin *et al.* (2005, 2006); Wang *et al.* (2007).



Experimental

Crystal data

$C_9H_8N_4O_3$
M_r = 220.19
Monoclinic, $P2_1/n$
a = 11.2344 (4) Å
b = 7.7197 (3) Å
c = 22.789 (1) Å
β = 94.730 (1)°
V = 1969.65 (14) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 296 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.977, T_{max} = 0.989
18061 measured reflections
3863 independent reflections
2540 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.134
S = 1.07
3863 reflections
290 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^{i}	0.93	2.59	3.367 (3)	141
C14—H14···O3^{i}	0.93	2.41	3.249 (3)	150
C17—H17···N4^{ii}	0.93	2.56	3.351 (3)	144

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LN2005).

References

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supporting information

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1-(4-Nitrophenoxymethyl)-1*H*-1,2,4-triazole

Jian Li

S1. Comment

The derivatives of 1,2,4-triazole are of great significance as pharmaceuticals, pesticides and high energetic materials. In recent years, the synthesis of energetic, polynitro and heterocyclic compounds have attracted considerable interest (Wang *et al.*, 2007; Jin *et al.*, 2005, 2006). This paper reports the crystal structure of the title 1,3,4-triazole derivative, (I).

The asymmetric unit of the title compound contains two independent molecules (Fig. 1). The dihedral angles formed by the triazole and benzene rings in the two independent molecules are 83.3 (3)° and 86.9 (4)°, respectively. The molecular packing involves weak C—H···N and C—H···O interactions (Table 1), and $\pi\cdots\pi$ stacking interactions of aromatic rings with the centroid to centroid distance being 3.745 (1) Å for adjacent benzene rings in pairs of molecules.

S2. Experimental

Anhydrous K_2CO_3(420 mg, 3.0 mmol) was added to a solution of *p*-nitrophenol (139 mg, 1.0 mmol) in anhydrous acetonitrile (30 ml). After stirring for 30 min at 333 K, 1-chloromethyl-1*H*-1, 2, 4-triazole (117 mg, 1.0 mmol) was added. The mixture was refluxed for 12 h. After cooling, a small amount of precipitate was removed by filtration. The residue was purified by column chromatography to obtain a white solid (yield 86.2%, m.p. 465 K decomp.). Suitable crystals were obtained by evaporation of an ethyl acetate solution of the product.

S3. Refinement

H atoms were positioned geometrically at distances of 0.93 Å (CH) and 0.97 Å (CH_2) from the parent C atoms; a riding model was used during the refinement process. The U_{iso} values were constrained to be $1.2U_{eq}$ of the carrier atom.

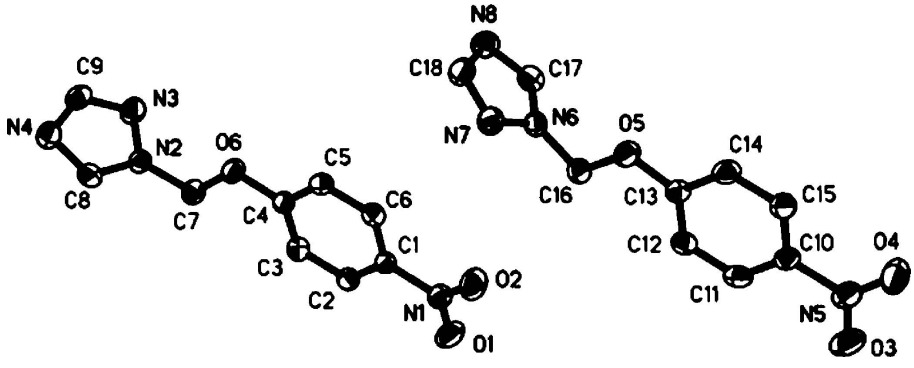

Figure 1

A view of the asymmetric unit of title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are omitted for clarity.

1-(4-Nitrophenoxymethyl)-1*H*-1,2,4-triazole

Crystal data

$C_9H_8N_4O_3$
$M_r = 220.19$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 11.2344$ (4) Å
$b = 7.7197$ (3) Å
$c = 22.789$ (1) Å
$\beta = 94.730$ (1)°
$V = 1969.65$ (14) Å^3
$Z = 8$
$F(000) = 912$
$D_x = 1.485$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2528 reflections
$\theta = 3.1$–$21.4°$
$\mu = 0.12$ mm^{-1}
$T = 296$ K
Block, colorless
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.977$, $T_{max} = 0.989$
18061 measured reflections
3863 independent reflections
2540 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.8°$
$h = -13 \rightarrow 13$
$k = -9 \rightarrow 9$
$l = -28 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.134$
$S = 1.07$
3863 reflections
290 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 0.0478P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ 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.

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.81377 (17)	0.3196 (3)	1.03182 (8)	0.0408 (5)
C2	0.93247 (17)	0.3426 (3)	1.04813 (8)	0.0458 (5)
H2	0.9670	0.4517	1.0461	0.055*
C3	1.00048 (18)	0.2022 (3)	1.06769 (9)	0.0462 (5)

H3	1.0817	0.2155	1.0783	0.055*
C4	0.94708 (17)	0.0410 (3)	1.07144 (8)	0.0413 (5)
C5	0.82669 (17)	0.0197 (3)	1.05410 (9)	0.0465 (5)
H5	0.7916	−0.0890	1.0559	0.056*
C6	0.75967 (18)	0.1595 (3)	1.03423 (9)	0.0452 (5)
H6	0.6789	0.1466	1.0225	0.054*
C7	1.12463 (17)	−0.0840 (3)	1.11700 (10)	0.0521 (6)
H7A	1.1301	0.0134	1.1440	0.063*
H7B	1.1768	−0.0623	1.0860	0.063*
C8	1.15858 (19)	−0.2774 (3)	1.20432 (10)	0.0543 (6)
H8	1.1336	−0.2011	1.2324	0.065*
C9	1.22169 (18)	−0.4899 (3)	1.16231 (11)	0.0572 (6)
H9	1.2515	−0.6003	1.1563	0.069*
C10	0.1692 (2)	0.7068 (3)	0.80842 (8)	0.0473 (5)
C11	0.2882 (2)	0.7309 (3)	0.82472 (9)	0.0533 (6)
H11	0.3213	0.8413	0.8243	0.064*
C12	0.35811 (18)	0.5906 (3)	0.84169 (9)	0.0494 (6)
H12	0.4390	0.6050	0.8529	0.059*
C13	0.30677 (17)	0.4276 (3)	0.84194 (9)	0.0440 (5)
C14	0.18569 (18)	0.4057 (3)	0.82638 (10)	0.0529 (6)
H14	0.1515	0.2962	0.8278	0.064*
C15	0.11677 (19)	0.5457 (3)	0.80901 (10)	0.0536 (6)
H15	0.0358	0.5323	0.7978	0.064*
C16	0.49184 (17)	0.2917 (3)	0.87293 (10)	0.0522 (6)
H16A	0.5060	0.3587	0.9088	0.063*
H16B	0.5322	0.3479	0.8421	0.063*
C17	0.58384 (17)	0.0123 (3)	0.84480 (10)	0.0543 (6)
H17	0.5990	0.0408	0.8065	0.065*
C18	0.5699 (2)	−0.1152 (3)	0.92397 (12)	0.0624 (6)
H18	0.5755	−0.2018	0.9524	0.075*
N1	0.74171 (17)	0.4702 (2)	1.01202 (8)	0.0516 (5)
N2	1.15923 (14)	−0.2405 (2)	1.14761 (7)	0.0444 (4)
N3	1.20085 (17)	−0.3790 (3)	1.11895 (8)	0.0605 (5)
N4	1.19720 (17)	−0.4338 (3)	1.21593 (9)	0.0617 (5)
N5	0.0937 (2)	0.8560 (3)	0.79082 (8)	0.0630 (6)
N6	0.53437 (14)	0.1182 (2)	0.88181 (7)	0.0460 (4)
N7	0.52429 (16)	0.0362 (3)	0.93374 (8)	0.0588 (5)
N8	0.60847 (16)	−0.1386 (3)	0.86990 (9)	0.0631 (6)
O1	0.79196 (15)	0.6084 (2)	1.00659 (8)	0.0747 (5)
O2	0.63420 (14)	0.4506 (2)	1.00168 (8)	0.0744 (5)
O3	0.13855 (18)	0.9998 (2)	0.79477 (7)	0.0843 (6)
O4	−0.01089 (19)	0.8306 (3)	0.77307 (8)	0.0874 (6)
O5	0.36738 (12)	0.27844 (18)	0.85648 (7)	0.0563 (4)
O6	1.00523 (12)	−0.10510 (18)	1.09272 (6)	0.0532 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0475 (11)	0.0415 (12)	0.0333 (11)	0.0041 (10)	0.0032 (9)	−0.0001 (9)
C2	0.0503 (12)	0.0425 (12)	0.0443 (12)	−0.0069 (10)	0.0025 (10)	0.0053 (10)
C3	0.0406 (11)	0.0508 (14)	0.0474 (13)	−0.0034 (10)	0.0042 (9)	0.0055 (10)
C4	0.0445 (11)	0.0418 (12)	0.0377 (11)	0.0039 (10)	0.0043 (9)	−0.0005 (10)
C5	0.0494 (12)	0.0384 (12)	0.0511 (13)	−0.0060 (10)	0.0008 (10)	−0.0018 (10)
C6	0.0419 (11)	0.0501 (14)	0.0434 (12)	−0.0017 (10)	0.0018 (9)	−0.0028 (10)
C7	0.0435 (12)	0.0524 (14)	0.0602 (14)	0.0039 (10)	0.0030 (10)	0.0046 (11)
C8	0.0630 (14)	0.0564 (16)	0.0435 (14)	−0.0004 (12)	0.0039 (11)	−0.0047 (11)
C9	0.0490 (13)	0.0460 (14)	0.0765 (17)	0.0087 (11)	0.0041 (12)	0.0014 (14)
C10	0.0656 (14)	0.0413 (13)	0.0356 (12)	0.0079 (11)	0.0083 (10)	−0.0034 (10)
C11	0.0730 (16)	0.0407 (13)	0.0469 (13)	−0.0105 (11)	0.0085 (11)	−0.0050 (10)
C12	0.0474 (12)	0.0472 (14)	0.0532 (13)	−0.0077 (10)	0.0022 (10)	−0.0052 (11)
C13	0.0452 (11)	0.0410 (13)	0.0462 (12)	0.0001 (10)	0.0065 (9)	−0.0038 (10)
C14	0.0477 (12)	0.0400 (13)	0.0710 (16)	−0.0056 (10)	0.0047 (11)	−0.0036 (11)
C15	0.0484 (12)	0.0510 (14)	0.0608 (15)	0.0015 (11)	0.0008 (11)	−0.0052 (11)
C16	0.0452 (12)	0.0528 (14)	0.0575 (14)	−0.0006 (10)	−0.0027 (10)	0.0005 (11)
C17	0.0420 (12)	0.0655 (16)	0.0559 (14)	0.0025 (11)	0.0069 (10)	−0.0078 (13)
C18	0.0598 (14)	0.0543 (16)	0.0716 (18)	0.0023 (12)	−0.0028 (13)	0.0067 (14)
N1	0.0583 (12)	0.0486 (12)	0.0478 (11)	0.0069 (10)	0.0038 (9)	−0.0010 (9)
N2	0.0447 (9)	0.0428 (11)	0.0460 (11)	0.0058 (8)	0.0052 (8)	0.0018 (9)
N3	0.0677 (12)	0.0589 (13)	0.0562 (12)	0.0249 (10)	0.0133 (10)	−0.0016 (10)
N4	0.0680 (13)	0.0552 (13)	0.0609 (13)	0.0003 (10)	−0.0007 (10)	0.0084 (11)
N5	0.0972 (17)	0.0528 (14)	0.0397 (11)	0.0174 (13)	0.0100 (11)	0.0012 (10)
N6	0.0450 (10)	0.0490 (11)	0.0433 (10)	0.0028 (8)	0.0000 (8)	0.0018 (9)
N7	0.0703 (12)	0.0585 (13)	0.0475 (12)	0.0035 (10)	0.0040 (9)	0.0055 (10)
N8	0.0540 (12)	0.0585 (14)	0.0766 (15)	0.0068 (10)	0.0034 (10)	−0.0082 (12)
O1	0.0813 (12)	0.0423 (10)	0.0994 (14)	0.0034 (9)	0.0008 (10)	0.0088 (9)
O2	0.0509 (10)	0.0748 (12)	0.0957 (13)	0.0124 (8)	−0.0050 (9)	0.0076 (10)
O3	0.1379 (17)	0.0431 (11)	0.0728 (13)	0.0136 (11)	0.0146 (11)	0.0049 (9)
O4	0.0864 (13)	0.0898 (15)	0.0835 (13)	0.0339 (11)	−0.0075 (11)	0.0022 (11)
O5	0.0418 (8)	0.0452 (9)	0.0807 (11)	−0.0004 (7)	−0.0024 (7)	0.0013 (8)
O6	0.0479 (8)	0.0434 (9)	0.0667 (10)	0.0016 (7)	−0.0057 (7)	0.0056 (8)

Geometric parameters (Å, º)

C1—C2	1.366 (3)	C11—C12	1.375 (3)
C1—C6	1.381 (3)	C11—H11	0.9300
C1—N1	1.466 (3)	C12—C13	1.384 (3)
C2—C3	1.379 (3)	C12—H12	0.9300
C2—H2	0.9300	C13—O5	1.365 (2)
C3—C4	1.387 (3)	C13—C14	1.387 (3)
C3—H3	0.9300	C14—C15	1.369 (3)
C4—O6	1.372 (2)	C14—H14	0.9300
C4—C5	1.387 (3)	C15—H15	0.9300
C5—C6	1.371 (3)	C16—O5	1.421 (2)

C5—H5	0.9300	C16—N6	1.431 (3)
C6—H6	0.9300	C16—H16A	0.9700
C7—O6	1.418 (2)	C16—H16B	0.9700
C7—N2	1.433 (3)	C17—N8	1.317 (3)
C7—H7A	0.9700	C17—N6	1.329 (3)
C7—H7B	0.9700	C17—H17	0.9300
C8—N4	1.303 (3)	C18—N7	1.302 (3)
C8—N2	1.324 (2)	C18—N8	1.352 (3)
C8—H8	0.9300	C18—H18	0.9300
C9—N3	1.314 (3)	N1—O1	1.218 (2)
C9—N4	1.346 (3)	N1—O2	1.221 (2)
C9—H9	0.9300	N2—N3	1.356 (2)
C10—C11	1.370 (3)	N5—O3	1.219 (3)
C10—C15	1.376 (3)	N5—O4	1.226 (3)
C10—N5	1.467 (3)	N6—N7	1.355 (2)

C2—C1—C6	121.91 (19)	O5—C13—C14	114.73 (18)
C2—C1—N1	118.85 (19)	C12—C13—C14	120.7 (2)
C6—C1—N1	119.23 (18)	C15—C14—C13	119.8 (2)
C1—C2—C3	119.2 (2)	C15—C14—H14	120.1
C1—C2—H2	120.4	C13—C14—H14	120.1
C3—C2—H2	120.4	C14—C15—C10	118.9 (2)
C2—C3—C4	119.62 (19)	C14—C15—H15	120.5
C2—C3—H3	120.2	C10—C15—H15	120.5
C4—C3—H3	120.2	O5—C16—N6	106.23 (16)
O6—C4—C3	124.31 (17)	O5—C16—H16A	110.5
O6—C4—C5	115.34 (18)	N6—C16—H16A	110.5
C3—C4—C5	120.34 (19)	O5—C16—H16B	110.5
C6—C5—C4	119.80 (19)	N6—C16—H16B	110.5
C6—C5—H5	120.1	H16A—C16—H16B	108.7
C4—C5—H5	120.1	N8—C17—N6	110.6 (2)
C5—C6—C1	119.09 (19)	N8—C17—H17	124.7
C5—C6—H6	120.5	N6—C17—H17	124.7
C1—C6—H6	120.5	N7—C18—N8	115.9 (2)
O6—C7—N2	107.66 (16)	N7—C18—H18	122.1
O6—C7—H7A	110.2	N8—C18—H18	122.1
N2—C7—H7A	110.2	O1—N1—O2	123.24 (19)
O6—C7—H7B	110.2	O1—N1—C1	118.48 (18)
N2—C7—H7B	110.2	O2—N1—C1	118.28 (19)
H7A—C7—H7B	108.5	C8—N2—N3	109.30 (18)
N4—C8—N2	111.6 (2)	C8—N2—C7	129.31 (19)
N4—C8—H8	124.2	N3—N2—C7	121.39 (17)
N2—C8—H8	124.2	C9—N3—N2	101.46 (18)
N3—C9—N4	115.9 (2)	C8—N4—C9	101.73 (19)
N3—C9—H9	122.1	O3—N5—O4	123.3 (2)
N4—C9—H9	122.1	O3—N5—C10	117.9 (2)
C11—C10—C15	121.9 (2)	O4—N5—C10	118.8 (2)
C11—C10—N5	119.8 (2)	C17—N6—N7	109.65 (18)

C15—C10—N5	118.3 (2)	C17—N6—C16	129.68 (19)
C10—C11—C12	119.4 (2)	N7—N6—C16	120.66 (18)
C10—C11—H11	120.3	C18—N7—N6	101.97 (19)
C12—C11—H11	120.3	C17—N8—C18	101.9 (2)
C11—C12—C13	119.25 (19)	N1—O2—H16A	132.4
C11—C12—H12	120.4	C13—O5—C16	117.61 (16)
C13—C12—H12	120.4	C4—O6—C7	116.82 (16)
O5—C13—C12	124.62 (18)		

C6—C1—C2—C3	−0.1 (3)	O6—C7—N2—C8	−96.5 (2)
N1—C1—C2—C3	178.99 (17)	O6—C7—N2—N3	84.1 (2)
C1—C2—C3—C4	−1.1 (3)	N4—C9—N3—N2	−0.1 (2)
C2—C3—C4—O6	−176.99 (18)	C8—N2—N3—C9	0.2 (2)
C2—C3—C4—C5	1.8 (3)	C7—N2—N3—C9	179.73 (17)
O6—C4—C5—C6	177.62 (18)	N2—C8—N4—C9	0.1 (2)
C3—C4—C5—C6	−1.3 (3)	N3—C9—N4—C8	0.0 (3)
C4—C5—C6—C1	0.1 (3)	C11—C10—N5—O3	−4.4 (3)
C2—C1—C6—C5	0.6 (3)	C15—C10—N5—O3	174.4 (2)
N1—C1—C6—C5	−178.46 (17)	C11—C10—N5—O4	175.75 (19)
C15—C10—C11—C12	0.6 (3)	C15—C10—N5—O4	−5.5 (3)
N5—C10—C11—C12	179.39 (18)	N8—C17—N6—N7	−0.4 (2)
C10—C11—C12—C13	0.0 (3)	N8—C17—N6—C16	−178.74 (19)
C11—C12—C13—O5	178.33 (19)	O5—C16—N6—C17	94.9 (2)
C11—C12—C13—C14	−1.2 (3)	O5—C16—N6—N7	−83.2 (2)
O5—C13—C14—C15	−177.77 (19)	N8—C18—N7—N6	−0.2 (2)
C12—C13—C14—C15	1.8 (3)	C17—N6—N7—C18	0.3 (2)
C13—C14—C15—C10	−1.2 (3)	C16—N6—N7—C18	178.84 (18)
C11—C10—C15—C14	0.0 (3)	N6—C17—N8—C18	0.3 (2)
N5—C10—C15—C14	−178.81 (19)	N7—C18—N8—C17	−0.1 (3)
C2—C1—N1—O1	5.4 (3)	C12—C13—O5—C16	0.5 (3)
C6—C1—N1—O1	−175.47 (19)	C14—C13—O5—C16	−179.93 (18)
C2—C1—N1—O2	−174.71 (18)	N6—C16—O5—C13	−176.10 (17)
C6—C1—N1—O2	4.4 (3)	C3—C4—O6—C7	5.8 (3)
N4—C8—N2—N3	−0.2 (2)	C5—C4—O6—C7	−173.07 (17)
N4—C8—N2—C7	−179.68 (19)	N2—C7—O6—C4	167.68 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	0.93	2.59	3.367 (3)	141
C14—H14···O3^{i}	0.93	2.41	3.249 (3)	150
C17—H17···N4^{ii}	0.93	2.56	3.351 (3)	144

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