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5-Methyl-1-(4-methylphenyl)-*N*′-[1-(1*H*-pyrrol-2-yl)ethylidene]-1*H*-1,2,3-triazole-4-carbohydrazide monohydrate

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Keywords: crystal structure; pyrrole; carbohydrazide.

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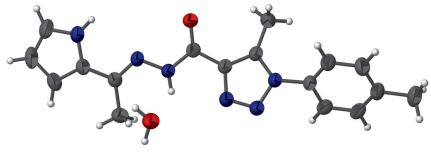
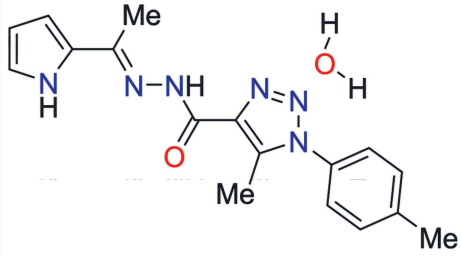
Structural data: full structural data are available from iucrdata.iucr.org

In the title hydrate, $C_{17}H_{18}N_6O\cdot H_2O$, the twist angles between the least-squares planes of the pyrolyl/methyltriazolyl/tolyl groups are 11.4 (2) and 7.9 (1)°, respectively. In the crystal, centrosymmetric tetramers (two organic molecules and two water molecules) are linked by N—H···O and O—H···O hydrogen bonds. Weak aromatic π–π stacking interactions between the triazolyl rings [centroid–centroid separation = 3.6422 (10) Å] link the tetramers.

3D view



Chemical scheme



Structure description

Arylidene carbohydrazides have various biological activities (Almasirad *et al.*, 2005; Bonacorso *et al.*, 2012; Hernández-Vázquez *et al.*, 2016; Leite *et al.*, 1999; Lima *et al.*, 2000). As part of our studies in this area, we now describe the synthesis and structure of the title hydrate.

The asymmetric unit consists of a 1,2,3-triazole-4-carbohydrazide molecule and a water molecule (Fig. 1). The twist angles between the least-squares planes of the pyrolyl/methyltriazolyl/tolyl groups are 11.4 (2) and 7.9 (1)°, respectively. In the crystal, the pyrolyl group donates an N—H···O hydrogen bond to the water molecule, which in turn donates O—H hydrogen bonds to two neighbouring molecules, thereby linking them (Table 1, Fig. 2) into a centrosymmetric tetramer. Organic molecules related by inversion symmetry are arranged in pairs with the centroids of their triazolyl rings 3.6422 (10) Å

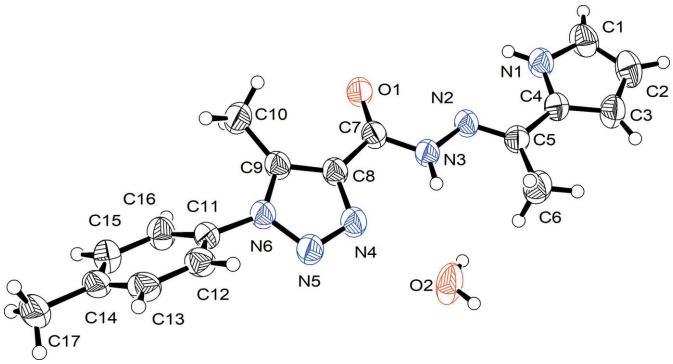


Figure 1
The molecular structure, showing 50% probability displacement ellipsoids.

apart. The pairs are stacked such that the closest distance between the centroids of triazolyl groups of neighbouring pairs is 3.967 (2) Å.

Synthesis and crystallization

The title compound (yield 85%) was synthesized from reaction of a mixture of 5-methyl-1-(4-methylphenyl)-1*H*-1,2,3-triazole-4-carbohydrazide and 1-(1*H*-pyrrol-2-yl)ethanone in boiling ethanol containing a few drops of acetic acid for 4 h. The crude product obtained was recrystallized from dimethylformamide solution to give colourless crystals. The water molecule of crystallization was presumably absorbed from the atmosphere.

Refinement

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

Funding information

MHA thanks King Abdulaziz City for Science and Technology (KACST), Saudi Arabia for financial support (award No. 020-0180).

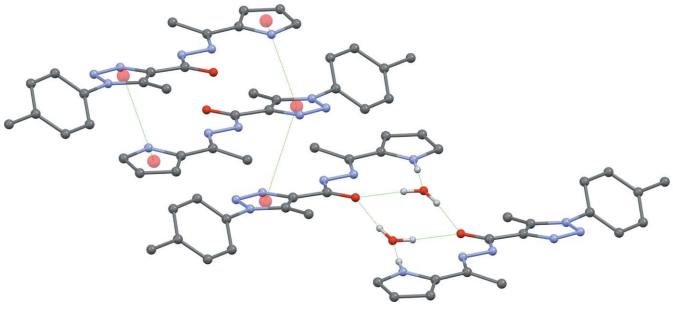


Figure 2
A segment of the crystal structure, showing N—H···O and O—H···O hydrogen bonds and centroid–centroid contacts as dashed lines. Some H atoms have been omitted for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2^{i}	0.86	1.98	2.838 (2)	176
O2—H1*O*···O1^{ii}	0.87 (4)	1.96 (4)	2.822 (2)	174 (3)
O2—H2*O*···N2^{i}	0.79 (4)	2.43 (4)	2.966 (3)	126 (3)
O2—H2*O*···O1^{i}	0.79 (4)	2.20 (4)	2.961 (2)	162 (3)

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x-1, y, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{18}N_6O\cdot H_2O$
M_r	340.39
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	7.3968 (8), 10.6475 (9), 12.7769 (13)
α, β, γ (°)	106.577 (9), 100.809 (9), 108.208 (9)
V (Å^3)	872.83 (16)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.26 × 0.18 × 0.15
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.497, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7305, 4129, 2871
R_{int}	0.022
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.699
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.155, 1.05
No. of reflections	4129
No. of parameters	237
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.27

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

References

Almasirad, A., Tajik, M., Bakhtiari, D., Shafiee, A., Abdollahi, M., Zamani, M. J., Khorasani, R. & Esmaily, H. (2005). *J. Pharm. Pharm. Sci.* **8**, 419–425.
Bonacorso, H. G., Cavinatto, S., Campos, P. T., Porte, L. M. F., Navarini, J., Paim, G. R., Martins, M. A. P., Zanatta, N. & Stuker, C. Z. (2012). *J. Fluor. Chem.* **135**, 303–314.
Cambridge Soft (2001). *CHEMDRAW Ultra*. Cambridge Soft Corporation, Cambridge, Massachusetts, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Hernández-Vázquez, E., Salgado-Barrera, S., Ramírez-Espinosa, J. J., Estrada-Soto, S. & Hernández-Luis, F. (2016). *Bioorg. Med. Chem.* **24**, 2298–2306.
Leite, L. F., Ramos, M. N., da Silva, J. B., Miranda, A. L., Fraga, C. A. & Barreiro, E. J. (1999). *Farmaco*, **54**, 747–757.
Lima, P. C., Lima, L. M., da Silva, K. C., Léda, P. H., de Miranda, A. L., Fraga, C. A. & Barreiro, E. J. (2000). *Eur. J. Med. Chem.* **35**, 187–203.

Rigaku OD (2015). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

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Crystal data

$C_{17}H_{18}N_6O·H_2O$
M_r = 340.39
Triclinic, $P\overline{1}$
a = 7.3968 (8) Å
b = 10.6475 (9) Å
c = 12.7769 (13) Å
α = 106.577 (9)°
β = 100.809 (9)°
γ = 108.208 (9)°
V = 872.83 (16) Å^3
Z = 2
$F(000)$ = 360
D_x = 1.295 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2273 reflections
θ = 3.4–28.7°
μ = 0.09 mm^{-1}
T = 296 K
Block, colourless
0.26 × 0.18 × 0.15 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.497, T_{max} = 1.000
7305 measured reflections
4129 independent reflections
2871 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 29.8°, θ_{min} = 3.0°
h = −9→9
k = −14→13
l = −16→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.155
S = 1.05
4129 reflections
237 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2 + 0.2675P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 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.

Refinement. Water H atoms were located on the difference Fourier map and refined freely. The rest of the H atoms were placed in calculated positions and refined using a riding model. Methyl C—H bonds were fixed at 0.96 Å, with displacement parameters 1.5 times U_{eq}(C), and were allowed to spin about the C—C bond. N—H bonds were fixed at 0.86 Å and aromatic C—H distances were set at 0.93 Å and their U_{iso} values set at 1.2 times the U_{eq} for the atoms to which they are bonded.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4498 (4)	0.5591 (2)	−0.34752 (19)	0.0624 (6)
H1	0.552068	0.614290	−0.367621	0.075*
C2	0.2509 (4)	0.5212 (3)	−0.3952 (2)	0.0674 (7)
H2	0.192987	0.545682	−0.453369	0.081*
C3	0.1493 (3)	0.4384 (2)	−0.34062 (18)	0.0582 (6)
H3	0.011555	0.397898	−0.355871	0.070*
C4	0.2908 (3)	0.4282 (2)	−0.26023 (15)	0.0449 (4)
C5	0.2718 (3)	0.3527 (2)	−0.18161 (15)	0.0435 (4)
C6	0.0678 (3)	0.2643 (3)	−0.1852 (2)	0.0661 (6)
H6A	0.050998	0.166304	−0.208278	0.099*
H6B	−0.030420	0.274780	−0.239134	0.099*
H6C	0.051649	0.295101	−0.110493	0.099*
C7	0.5842 (3)	0.28246 (19)	0.01528 (15)	0.0427 (4)
C8	0.5431 (3)	0.19870 (19)	0.08797 (15)	0.0437 (4)
C9	0.6700 (3)	0.1633 (2)	0.15650 (15)	0.0447 (4)
C10	0.8839 (3)	0.1866 (3)	0.1746 (2)	0.0644 (6)
H10A	0.965436	0.277622	0.233966	0.097*
H10B	0.915867	0.184061	0.104786	0.097*
H10C	0.908864	0.113237	0.196794	0.097*
C11	0.5936 (3)	0.02833 (19)	0.28757 (15)	0.0423 (4)
C12	0.4664 (3)	−0.1064 (2)	0.27027 (16)	0.0473 (5)
H12	0.357886	−0.158025	0.204142	0.057*
C13	0.5012 (3)	−0.1642 (2)	0.35192 (17)	0.0510 (5)
H13	0.414885	−0.255287	0.340156	0.061*
C14	0.6612 (3)	−0.0901 (2)	0.45079 (17)	0.0493 (5)
C15	0.7877 (3)	0.0454 (2)	0.46619 (17)	0.0537 (5)
H15	0.897338	0.096469	0.531771	0.064*
C16	0.7543 (3)	0.1060 (2)	0.38601 (17)	0.0514 (5)
H16	0.838664	0.197805	0.398139	0.062*
C17	0.6964 (4)	−0.1568 (3)	0.5383 (2)	0.0680 (6)
H17A	0.574689	−0.194456	0.555808	0.102*
H17B	0.797874	−0.086174	0.606917	0.102*
H17C	0.738952	−0.232303	0.507897	0.102*
N1	0.4733 (3)	0.50299 (17)	−0.26600 (14)	0.0512 (4)

H1A	0.586128	0.512927	−0.224096	0.061*
N2	0.4359 (2)	0.36382 (16)	−0.11682 (13)	0.0447 (4)
N3	0.4194 (2)	0.28847 (17)	−0.04530 (13)	0.0463 (4)
H3A	0.304451	0.245452	−0.039329	0.056*
N4	0.3558 (2)	0.14459 (19)	0.09563 (14)	0.0528 (4)
N5	0.3573 (2)	0.07814 (19)	0.16659 (15)	0.0539 (4)
N6	0.5496 (2)	0.08967 (17)	0.20462 (13)	0.0455 (4)
O1	0.75210 (19)	0.33899 (15)	0.00833 (11)	0.0534 (4)
O2	0.1638 (3)	0.4799 (3)	0.1289 (2)	0.1062 (9)
H1O	0.036 (6)	0.435 (4)	0.097 (3)	0.130 (13)*
H2O	0.211 (5)	0.529 (4)	0.097 (3)	0.109 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0743 (16)	0.0615 (13)	0.0618 (13)	0.0252 (12)	0.0203 (11)	0.0391 (11)
C2	0.0841 (18)	0.0699 (15)	0.0594 (13)	0.0369 (13)	0.0114 (12)	0.0388 (12)
C3	0.0546 (13)	0.0656 (14)	0.0585 (12)	0.0275 (11)	0.0077 (10)	0.0301 (11)
C4	0.0470 (11)	0.0474 (11)	0.0436 (10)	0.0207 (9)	0.0111 (8)	0.0205 (8)
C5	0.0409 (10)	0.0469 (10)	0.0433 (9)	0.0165 (8)	0.0106 (8)	0.0196 (8)
C6	0.0405 (12)	0.0849 (16)	0.0720 (14)	0.0128 (11)	0.0108 (10)	0.0445 (13)
C7	0.0401 (10)	0.0453 (10)	0.0398 (9)	0.0114 (8)	0.0089 (7)	0.0192 (8)
C8	0.0391 (10)	0.0479 (11)	0.0435 (9)	0.0120 (8)	0.0099 (7)	0.0233 (8)
C9	0.0410 (10)	0.0489 (11)	0.0462 (10)	0.0129 (8)	0.0121 (8)	0.0262 (8)
C10	0.0452 (12)	0.0883 (17)	0.0806 (15)	0.0278 (11)	0.0224 (11)	0.0565 (14)
C11	0.0425 (10)	0.0481 (10)	0.0459 (10)	0.0197 (8)	0.0165 (8)	0.0268 (8)
C12	0.0466 (11)	0.0469 (11)	0.0493 (10)	0.0147 (9)	0.0176 (8)	0.0212 (9)
C13	0.0554 (12)	0.0463 (11)	0.0635 (12)	0.0203 (9)	0.0286 (10)	0.0302 (10)
C14	0.0599 (12)	0.0588 (12)	0.0545 (11)	0.0358 (10)	0.0305 (10)	0.0342 (10)
C15	0.0567 (12)	0.0567 (12)	0.0508 (11)	0.0242 (10)	0.0111 (9)	0.0252 (10)
C16	0.0511 (12)	0.0452 (11)	0.0563 (11)	0.0137 (9)	0.0104 (9)	0.0256 (9)
C17	0.0860 (17)	0.0842 (17)	0.0734 (15)	0.0506 (14)	0.0406 (13)	0.0550 (13)
N1	0.0508 (10)	0.0571 (10)	0.0542 (9)	0.0212 (8)	0.0144 (7)	0.0332 (8)
N2	0.0423 (9)	0.0525 (9)	0.0456 (8)	0.0172 (7)	0.0126 (7)	0.0287 (7)
N3	0.0361 (8)	0.0582 (10)	0.0503 (9)	0.0141 (7)	0.0125 (7)	0.0333 (8)
N4	0.0420 (9)	0.0660 (11)	0.0572 (10)	0.0171 (8)	0.0131 (7)	0.0382 (9)
N5	0.0401 (9)	0.0675 (11)	0.0618 (10)	0.0165 (8)	0.0142 (7)	0.0405 (9)
N6	0.0388 (9)	0.0521 (9)	0.0504 (9)	0.0147 (7)	0.0123 (7)	0.0298 (7)
O1	0.0375 (7)	0.0699 (9)	0.0561 (8)	0.0135 (7)	0.0118 (6)	0.0375 (7)
O2	0.0396 (10)	0.147 (2)	0.1405 (19)	0.0047 (11)	0.0041 (11)	0.1141 (18)

Geometric parameters (Å, º)

C1—N1	1.351 (2)	C10—H10C	0.9600
C1—C2	1.360 (3)	C11—C12	1.375 (3)
C1—H1	0.9300	C11—C16	1.382 (3)
C2—C3	1.400 (3)	C11—N6	1.433 (2)
C2—H2	0.9300	C12—C13	1.377 (3)

C3—C4	1.377 (3)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.380 (3)
C4—N1	1.364 (3)	C13—H13	0.9300
C4—C5	1.455 (2)	C14—C15	1.386 (3)
C5—N2	1.285 (2)	C14—C17	1.511 (3)
C5—C6	1.492 (3)	C15—C16	1.382 (3)
C6—H6A	0.9600	C15—H15	0.9300
C6—H6B	0.9600	C16—H16	0.9300
C6—H6C	0.9600	C17—H17A	0.9600
C7—O1	1.232 (2)	C17—H17B	0.9600
C7—N3	1.346 (2)	C17—H17C	0.9600
C7—C8	1.470 (2)	N1—H1A	0.8600
C8—N4	1.359 (2)	N2—N3	1.376 (2)
C8—C9	1.375 (2)	N3—H3A	0.8600
C9—N6	1.353 (2)	N4—N5	1.300 (2)
C9—C10	1.484 (3)	N5—N6	1.368 (2)
C10—H10A	0.9600	O2—H1O	0.87 (4)
C10—H10B	0.9600	O2—H2O	0.79 (4)

N1—C1—C2	108.3 (2)	C12—C11—N6	118.61 (16)
N1—C1—H1	125.8	C16—C11—N6	120.64 (16)
C2—C1—H1	125.8	C11—C12—C13	119.31 (18)
C1—C2—C3	107.43 (18)	C11—C12—H12	120.3
C1—C2—H2	126.3	C13—C12—H12	120.3
C3—C2—H2	126.3	C12—C13—C14	121.59 (18)
C4—C3—C2	107.4 (2)	C12—C13—H13	119.2
C4—C3—H3	126.3	C14—C13—H13	119.2
C2—C3—H3	126.3	C13—C14—C15	118.07 (17)
N1—C4—C3	107.16 (17)	C13—C14—C17	120.34 (19)
N1—C4—C5	121.31 (16)	C15—C14—C17	121.6 (2)
C3—C4—C5	131.50 (19)	C16—C15—C14	121.31 (19)
N2—C5—C4	116.18 (17)	C16—C15—H15	119.3
N2—C5—C6	125.02 (17)	C14—C15—H15	119.3
C4—C5—C6	118.75 (16)	C11—C16—C15	119.06 (18)
C5—C6—H6A	109.5	C11—C16—H16	120.5
C5—C6—H6B	109.5	C15—C16—H16	120.5
H6A—C6—H6B	109.5	C14—C17—H17A	109.5
C5—C6—H6C	109.5	C14—C17—H17B	109.5
H6A—C6—H6C	109.5	H17A—C17—H17B	109.5
H6B—C6—H6C	109.5	C14—C17—H17C	109.5
O1—C7—N3	123.18 (16)	H17A—C17—H17C	109.5
O1—C7—C8	123.42 (16)	H17B—C17—H17C	109.5
N3—C7—C8	113.38 (16)	C1—N1—C4	109.67 (17)
N4—C8—C9	109.63 (15)	C1—N1—H1A	125.2
N4—C8—C7	120.37 (16)	C4—N1—H1A	125.2
C9—C8—C7	129.99 (17)	C5—N2—N3	116.60 (16)
N6—C9—C8	103.14 (16)	C7—N3—N2	119.63 (15)
N6—C9—C10	124.59 (16)	C7—N3—H3A	120.2

C8—C9—C10	132.18 (17)	N2—N3—H3A	120.2
C9—C10—H10A	109.5	N5—N4—C8	109.18 (15)
C9—C10—H10B	109.5	N4—N5—N6	106.59 (15)
H10A—C10—H10B	109.5	C9—N6—N5	111.46 (14)
C9—C10—H10C	109.5	C9—N6—C11	130.64 (16)
H10A—C10—H10C	109.5	N5—N6—C11	117.88 (14)
H10B—C10—H10C	109.5	H1O—O2—H2O	111 (3)
C12—C11—C16	120.66 (16)		

N1—C1—C2—C3	−0.1 (3)	N6—C11—C16—C15	177.54 (18)
C1—C2—C3—C4	0.0 (3)	C14—C15—C16—C11	−1.4 (3)
C2—C3—C4—N1	0.1 (2)	C2—C1—N1—C4	0.2 (3)
C2—C3—C4—C5	−178.0 (2)	C3—C4—N1—C1	−0.2 (2)
N1—C4—C5—N2	1.6 (3)	C5—C4—N1—C1	178.16 (18)
C3—C4—C5—N2	179.5 (2)	C4—C5—N2—N3	−177.59 (16)
N1—C4—C5—C6	−175.7 (2)	C6—C5—N2—N3	−0.5 (3)
C3—C4—C5—C6	2.2 (3)	O1—C7—N3—N2	−1.8 (3)
O1—C7—C8—N4	177.01 (19)	C8—C7—N3—N2	179.80 (15)
N3—C7—C8—N4	−4.5 (3)	C5—N2—N3—C7	172.56 (17)
O1—C7—C8—C9	−2.0 (3)	C9—C8—N4—N5	0.8 (2)
N3—C7—C8—C9	176.40 (19)	C7—C8—N4—N5	−178.43 (17)
N4—C8—C9—N6	−1.0 (2)	C8—N4—N5—N6	−0.2 (2)
C7—C8—C9—N6	178.14 (19)	C8—C9—N6—N5	0.9 (2)
N4—C8—C9—C10	175.6 (2)	C10—C9—N6—N5	−176.1 (2)
C7—C8—C9—C10	−5.2 (4)	C8—C9—N6—C11	−177.44 (18)
C16—C11—C12—C13	−0.5 (3)	C10—C9—N6—C11	5.6 (3)
N6—C11—C12—C13	−176.89 (17)	N4—N5—N6—C9	−0.4 (2)
C11—C12—C13—C14	−0.1 (3)	N4—N5—N6—C11	178.13 (16)
C12—C13—C14—C15	−0.1 (3)	C12—C11—N6—C9	−136.0 (2)
C12—C13—C14—C17	−179.51 (19)	C16—C11—N6—C9	47.6 (3)
C13—C14—C15—C16	0.8 (3)	C12—C11—N6—N5	45.8 (2)
C17—C14—C15—C16	−179.7 (2)	C16—C11—N6—N5	−130.6 (2)
C12—C11—C16—C15	1.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2^{i}	0.86	1.98	2.838 (2)	176
O2—H1*O*···O1^{ii}	0.87 (4)	1.96 (4)	2.822 (2)	174 (3)
O2—H2*O*···N2^{i}	0.79 (4)	2.43 (4)	2.966 (3)	126 (3)
O2—H2*O*···O1^{i}	0.79 (4)	2.20 (4)	2.961 (2)	162 (3)

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