IUCrData

ISSN 2414-3146

5-Methyl-*N*′-(5-methyl-1-phenyl-1*H*-1,2,3-triazole-4-carbonyl)-1-phenyl-1*H*-1,2,3-triazole-4-carbohydrazide

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Received 8 March 2018
Accepted 12 March 2018

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

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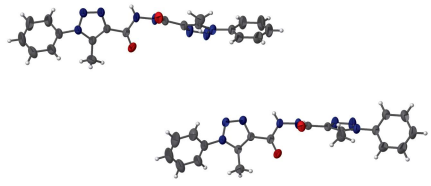
Keywords: crystal structure; 1,2,3-triazole; carbohydrazide.

CCDC reference: 1829173

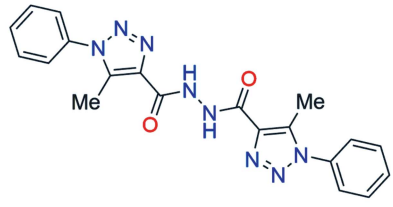
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{20}H_{18}N_8O_2$, comprises one complete molecule and a half molecule completed by crystallographic twofold symmetry leading to Z = 12. The dihedral angles between the planes of the linked phenyl and methyltriazolyl groups are 69.48 (5) and 44.85 (9)° for the first molecule and 42.88 (9)° for the second. The conformations of the diformyl hydrazyl groups of the molecules are similar as indicated by C—N—N—C torsion angles of −83.4 (2) and −86.4 (3)°. In the crystal, neighbouring molecules are linked by pairs of N—H···O hydrogen bonds to form independent columns propagating parallel to the *c*-axis direction.

3D view



Chemical scheme



Structure description

N,*N*′-Diacylhydrazines are precursors for heterocycles such as 1,3,4-oxadiazoles (Abdel-Wahab *et al.*, 2017). Treatment of acid hydrazides with an oxidizing agent gives *N*,*N*′-diacylhydrazines (Nikolić *et al.*, 2017; Mogilaiah *et al.*, 2003; Prakash *et al.*, 1997). As part of our studies in this area, we now describe the crystal structure of the title compound.

The asymmetric unit comprises one and a half molecules (Fig. 1). The second molecule is completed by crystallographic twofold symmetry. The dihedral angles between the planes of the linked phenyl and methyltriazolyl groups are 69.48 (5)° and 44.85 (9)° for the first molecule and 42.88 (9)° for the second. The conformations of the diformyl

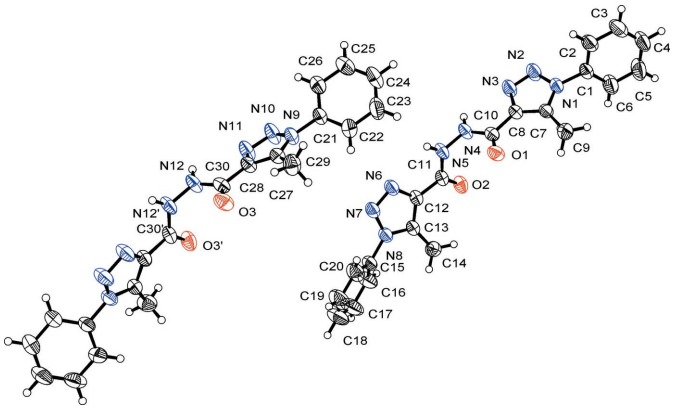


Figure 1
The molecular structure showing 50% displacement ellipsoids. Primed and unlabelled atoms are generated by the symmetry operation $1 - x, y, \frac{1}{2} - z$.

hydrazyl groups of the two molecules are similar as indicated by the C—N—N—C torsion angles of −83.4 (2)° and −86.4 (3)°. The dihedral angle between the C7 and C13 triazole rings in the first molecule is 63.65 (10) and the equivalent angle between the symmetry-related C27 rings in the second molecule is 61.80 (4)°.

Neighbouring molecules in the crystal structure are linked by pairs of N—H···O hydrogen bonds (Table 1), forming columns parallel to the *c*-axis direction The two types of molecule form separate columns that alternate along the *a*-axis direction (Fig. 2).

Synthesis and crystallization

The synthesis of the title compound has already been reported (Abdel-Wahab *et al.*, 2017). Yellow needles of the title compound were recrystallized from dimethylformamide solution (yield = 72%; m.p. 279–280°C).

Refinement

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O1^{i}	0.86	2.24	2.9412 (19)	139
N5—H5*A*···O2^{ii}	0.86	2.23	2.9395 (19)	140
N12—H12···O3^{iii}	0.86	2.28	3.098 (2)	158

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{18}N_8O_2$
M_r	402.42
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	296
a, *b*, *c* (Å)	61.5399 (18), 11.8988 (4), 8.2661 (3)
β (°)	93.301 (3)
V (Å^3)	6042.8 (3)
Z	12
Radiation type	Mo *K*α
μ (mm^{-1})	0.09
Crystal size (mm)	0.36 × 0.17 × 0.08
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*, Rigaku OD, 2015)
T_{min}, T_{max}	0.583, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28646, 7636, 5320
R_{int}	0.025
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.701
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.052, 0.162, 1.06
No. of reflections	7636
No. of parameters	410
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.24

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).

Funding information

The project was supported by King Saud University, Deanship of Scientific Research, Research Chairs.

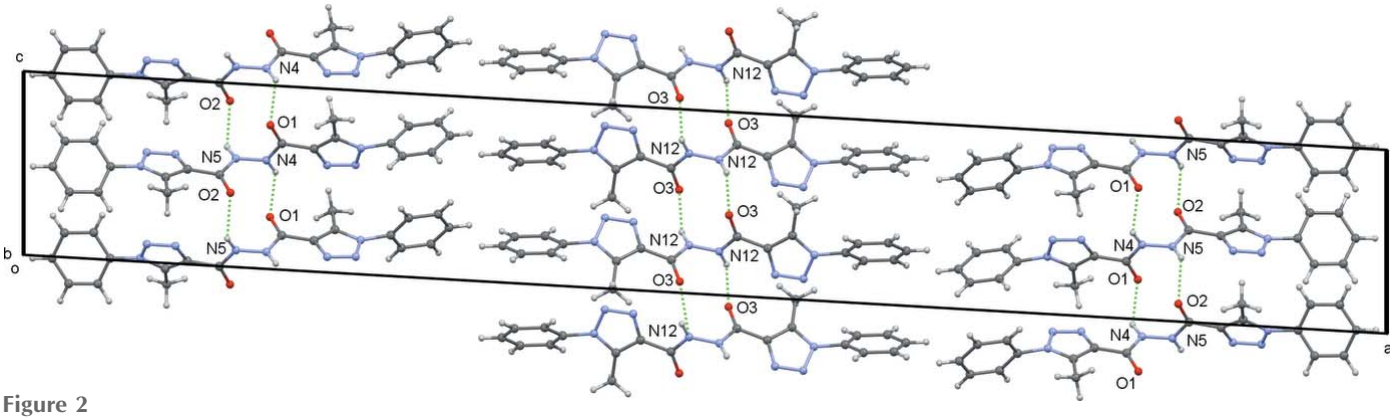


Figure 2
A segment of the crystal structure viewed down the *b* axis showing N—H···O hydrogen-bonding contacts leading to [001] chains.

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full crystallographic data

IUCrData (2018). **3**, x180424 [https://doi.org/10.1107/S2414314618004248]

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Crystal data

$C_{20}H_{18}N_8O_2$
M_r = 402.42
Monoclinic, *C*2/*c*
a = 61.5399 (18) Å
b = 11.8988 (4) Å
c = 8.2661 (3) Å
β = 93.301 (3)°
V = 6042.8 (3) Å^3
Z = 12
F(000) = 2520
D_x = 1.327 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 7925 reflections
θ = 3.3–29.3°
μ = 0.09 mm^{-1}
T = 296 K
Needle, yellow
0.36 × 0.17 × 0.08 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} = 0.583, T_{max} = 1.000
28646 measured reflections
7636 independent reflections
5320 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 29.9°, θ_{min} = 3.0°
h = −86→79
k = −16→16
l = −11→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.162
S = 1.06
7636 reflections
410 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0711P)^2 + 3.1965P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00114 (19)

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. All hydrogen atoms were placed in calculated positions and refined using a riding model. Aromatic C—H distances were set to 0.93\%A and their U(iso) set to 1.2 times the U_{eq} for the atoms to which they are bonded. Methyl groups were allowed to rotate about the C—C bond and C—H distances were set to 0.96\%A with U(iso) set to 1.5 times the U_{eq} for the C atoms to which they are bonded. The N—H bond was set to 0.86 Å and U_{iso}(H) set to 1.2 times U_{eq} (N).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.22978 (2)	0.37333 (15)	0.7766 (2)	0.0463 (4)
C2	0.21677 (3)	0.44007 (18)	0.6775 (3)	0.0629 (5)
H2	0.222337	0.504302	0.630957	0.075*
C3	0.19509 (3)	0.4103 (2)	0.6476 (3)	0.0772 (7)
H3	0.186076	0.454780	0.579953	0.093*
C4	0.18692 (3)	0.3164 (2)	0.7165 (3)	0.0738 (6)
H4	0.172289	0.298191	0.698205	0.089*
C5	0.20016 (3)	0.2491 (2)	0.8123 (3)	0.0787 (7)
H5	0.194609	0.184275	0.857403	0.094*
C6	0.22191 (3)	0.27693 (19)	0.8426 (3)	0.0682 (6)
H6	0.231025	0.230779	0.906967	0.082*
C7	0.27078 (2)	0.36356 (13)	0.7642 (2)	0.0403 (3)
C8	0.28629 (2)	0.43569 (13)	0.83050 (19)	0.0398 (3)
C9	0.27244 (3)	0.26166 (16)	0.6632 (3)	0.0596 (5)
H9A	0.258973	0.220841	0.661961	0.089*
H9B	0.284030	0.214962	0.707488	0.089*
H9C	0.275385	0.283020	0.554648	0.089*
C10	0.30996 (2)	0.43355 (14)	0.81230 (19)	0.0400 (3)
C11	0.35563 (2)	0.43823 (14)	1.00094 (19)	0.0410 (4)
C12	0.37925 (2)	0.44678 (14)	0.98102 (19)	0.0405 (3)
C13	0.39533 (2)	0.37223 (14)	1.03065 (19)	0.0405 (3)
C14	0.39412 (3)	0.26250 (15)	1.1149 (2)	0.0547 (4)
H14A	0.406393	0.217129	1.090101	0.082*
H14B	0.380918	0.224675	1.079264	0.082*
H14C	0.394262	0.274683	1.229725	0.082*
C15	0.43574 (3)	0.38279 (15)	0.9912 (2)	0.0496 (4)
C16	0.44469 (3)	0.3415 (2)	1.1341 (3)	0.0709 (6)
H16	0.436481	0.337511	1.224957	0.085*
C17	0.46606 (4)	0.3057 (3)	1.1423 (4)	0.0966 (9)
H17	0.472198	0.276129	1.238498	0.116*
C18	0.47825 (4)	0.3137 (3)	1.0095 (5)	0.0988 (9)
H18	0.492634	0.289331	1.015520	0.119*
C19	0.46925 (4)	0.3576 (3)	0.8671 (4)	0.0924 (9)
H19	0.477671	0.364003	0.777621	0.111*
C20	0.44778 (3)	0.3923 (2)	0.8559 (3)	0.0682 (6)

H20	0.441576	0.421280	0.759477	0.082*
C21	0.60369 (3)	0.87144 (15)	0.2703 (2)	0.0499 (4)
C22	0.61242 (3)	0.77039 (17)	0.3228 (3)	0.0573 (5)
H22	0.603357	0.711174	0.348183	0.069*
C23	0.63484 (3)	0.7577 (2)	0.3373 (3)	0.0714 (6)
H23	0.640836	0.689795	0.373190	0.086*
C24	0.64812 (3)	0.8442 (2)	0.2995 (4)	0.0905 (8)
H24	0.663156	0.835202	0.309213	0.109*
C25	0.63926 (3)	0.9448 (2)	0.2467 (5)	0.1052 (11)
H25	0.648369	1.003664	0.220610	0.126*
C26	0.61691 (3)	0.95940 (19)	0.2322 (4)	0.0810 (8)
H26	0.610951	1.027625	0.197199	0.097*
C27	0.56458 (2)	0.86275 (14)	0.3473 (2)	0.0426 (4)
C28	0.54653 (2)	0.91029 (14)	0.2699 (2)	0.0431 (4)
C29	0.56739 (3)	0.79950 (18)	0.5004 (2)	0.0601 (5)
H29A	0.567458	0.720405	0.477553	0.090*
H29B	0.555601	0.816576	0.567532	0.090*
H29C	0.580926	0.820337	0.555824	0.090*
C30	0.52413 (2)	0.91587 (15)	0.3236 (2)	0.0453 (4)
N1	0.25201 (2)	0.40700 (12)	0.81303 (18)	0.0450 (3)
N2	0.25575 (2)	0.50136 (14)	0.9052 (2)	0.0619 (5)
N3	0.27670 (2)	0.51714 (14)	0.9151 (2)	0.0565 (4)
N4	0.32124 (2)	0.50774 (13)	0.90749 (17)	0.0466 (3)
H4A	0.314472	0.552915	0.968324	0.056*
N5	0.34366 (2)	0.51120 (13)	0.90730 (18)	0.0468 (3)
H5A	0.349965	0.559343	0.848150	0.056*
N6	0.38802 (2)	0.53479 (13)	0.90331 (19)	0.0511 (4)
N7	0.40897 (2)	0.52009 (13)	0.9023 (2)	0.0536 (4)
N8	0.41358 (2)	0.42055 (12)	0.97963 (17)	0.0442 (3)
N9	0.58066 (2)	0.88693 (12)	0.24842 (18)	0.0469 (3)
N10	0.57279 (2)	0.94466 (15)	0.1149 (2)	0.0624 (5)
N11	0.55203 (2)	0.95812 (15)	0.12926 (19)	0.0578 (4)
N12	0.51107 (2)	0.98835 (14)	0.23792 (18)	0.0525 (4)
H12	0.516383	1.033741	0.169530	0.063*
O1	0.31841 (2)	0.37162 (11)	0.71613 (15)	0.0521 (3)
O2	0.34779 (2)	0.37352 (11)	1.09605 (15)	0.0516 (3)
O3	0.51812 (2)	0.86215 (12)	0.43867 (16)	0.0587 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0314 (7)	0.0552 (10)	0.0526 (10)	−0.0040 (7)	0.0047 (7)	−0.0018 (8)
C2	0.0383 (9)	0.0689 (12)	0.0812 (14)	−0.0015 (8)	0.0024 (9)	0.0135 (11)
C3	0.0394 (10)	0.0916 (16)	0.0993 (18)	0.0040 (10)	−0.0081 (10)	0.0130 (14)
C4	0.0346 (9)	0.0895 (16)	0.0970 (17)	−0.0123 (10)	0.0010 (10)	−0.0048 (14)
C5	0.0546 (12)	0.0879 (16)	0.0931 (17)	−0.0294 (11)	0.0001 (11)	0.0166 (13)
C6	0.0505 (10)	0.0772 (14)	0.0755 (14)	−0.0169 (10)	−0.0081 (9)	0.0221 (11)
C7	0.0336 (7)	0.0433 (8)	0.0439 (9)	0.0005 (6)	0.0009 (6)	0.0035 (7)

C8	0.0317 (7)	0.0466 (8)	0.0413 (8)	0.0007 (6)	0.0023 (6)	−0.0003 (7)
C9	0.0502 (10)	0.0512 (10)	0.0772 (14)	−0.0021 (8)	0.0016 (9)	−0.0140 (9)
C10	0.0330 (7)	0.0472 (8)	0.0399 (8)	0.0024 (6)	0.0025 (6)	0.0050 (7)
C11	0.0337 (7)	0.0514 (9)	0.0379 (8)	−0.0059 (7)	0.0032 (6)	−0.0044 (7)
C12	0.0325 (7)	0.0501 (9)	0.0389 (8)	−0.0047 (6)	0.0016 (6)	0.0018 (7)
C13	0.0343 (7)	0.0482 (9)	0.0392 (8)	−0.0029 (6)	0.0030 (6)	−0.0029 (7)
C14	0.0502 (10)	0.0510 (10)	0.0634 (12)	0.0016 (8)	0.0080 (8)	0.0086 (9)
C15	0.0332 (8)	0.0532 (10)	0.0629 (11)	0.0023 (7)	0.0063 (7)	−0.0082 (8)
C16	0.0448 (10)	0.0916 (16)	0.0760 (15)	0.0142 (10)	0.0014 (10)	0.0094 (12)
C17	0.0512 (12)	0.117 (2)	0.120 (2)	0.0285 (14)	−0.0035 (14)	0.0139 (18)
C18	0.0447 (12)	0.105 (2)	0.147 (3)	0.0245 (13)	0.0095 (15)	−0.017 (2)
C19	0.0521 (12)	0.112 (2)	0.116 (2)	0.0062 (13)	0.0330 (14)	−0.0272 (18)
C20	0.0500 (10)	0.0825 (14)	0.0735 (14)	−0.0001 (10)	0.0175 (10)	−0.0121 (11)
C21	0.0314 (7)	0.0540 (10)	0.0641 (11)	0.0051 (7)	0.0016 (7)	−0.0039 (8)
C22	0.0462 (9)	0.0574 (11)	0.0679 (12)	0.0101 (8)	−0.0002 (8)	0.0007 (9)
C23	0.0505 (11)	0.0766 (14)	0.0860 (16)	0.0242 (10)	−0.0061 (10)	−0.0014 (12)
C24	0.0347 (10)	0.0980 (18)	0.138 (2)	0.0130 (11)	−0.0053 (12)	−0.0087 (17)
C25	0.0391 (11)	0.0823 (17)	0.195 (3)	−0.0061 (11)	0.0125 (15)	0.0065 (19)
C26	0.0388 (10)	0.0608 (12)	0.144 (2)	0.0033 (9)	0.0096 (12)	0.0089 (14)
C27	0.0355 (7)	0.0455 (8)	0.0471 (9)	−0.0008 (6)	0.0045 (7)	−0.0002 (7)
C28	0.0320 (7)	0.0529 (9)	0.0445 (9)	−0.0021 (7)	0.0036 (6)	0.0050 (7)
C29	0.0586 (11)	0.0672 (12)	0.0548 (11)	0.0111 (9)	0.0057 (9)	0.0127 (9)
C30	0.0321 (7)	0.0576 (10)	0.0465 (9)	−0.0072 (7)	0.0048 (7)	−0.0007 (8)
N1	0.0315 (6)	0.0494 (8)	0.0542 (8)	−0.0036 (6)	0.0034 (6)	−0.0026 (6)
N2	0.0357 (7)	0.0674 (10)	0.0834 (12)	−0.0037 (7)	0.0106 (7)	−0.0255 (9)
N3	0.0338 (7)	0.0651 (9)	0.0712 (11)	−0.0041 (6)	0.0081 (7)	−0.0212 (8)
N4	0.0272 (6)	0.0632 (9)	0.0496 (8)	−0.0012 (6)	0.0034 (6)	−0.0075 (7)
N5	0.0265 (6)	0.0646 (9)	0.0494 (8)	−0.0048 (6)	0.0024 (6)	0.0076 (7)
N6	0.0341 (7)	0.0573 (9)	0.0622 (10)	−0.0013 (6)	0.0047 (6)	0.0124 (7)
N7	0.0339 (7)	0.0572 (9)	0.0702 (10)	−0.0026 (6)	0.0076 (7)	0.0125 (8)
N8	0.0332 (6)	0.0499 (8)	0.0495 (8)	−0.0001 (6)	0.0040 (6)	0.0014 (6)
N9	0.0321 (6)	0.0553 (8)	0.0535 (8)	0.0055 (6)	0.0039 (6)	0.0077 (7)
N10	0.0353 (7)	0.0872 (12)	0.0656 (10)	0.0123 (7)	0.0118 (7)	0.0286 (9)
N11	0.0325 (7)	0.0834 (11)	0.0582 (10)	0.0094 (7)	0.0094 (6)	0.0211 (8)
N12	0.0261 (6)	0.0760 (10)	0.0563 (9)	0.0002 (6)	0.0091 (6)	0.0088 (8)
O1	0.0395 (6)	0.0617 (8)	0.0555 (7)	0.0077 (5)	0.0056 (5)	−0.0080 (6)
O2	0.0408 (6)	0.0638 (8)	0.0507 (7)	−0.0097 (5)	0.0077 (5)	0.0071 (6)
O3	0.0441 (6)	0.0733 (9)	0.0598 (8)	−0.0107 (6)	0.0123 (6)	0.0114 (7)

Geometric parameters (Å, º)

C1—C2	1.366 (3)	C18—C19	1.375 (4)
C1—C6	1.371 (3)	C18—H18	0.9300
C1—N1	1.4403 (19)	C19—C20	1.383 (3)
C2—C3	1.389 (3)	C19—H19	0.9300
C2—H2	0.9300	C20—H20	0.9300
C3—C4	1.364 (3)	C21—C26	1.373 (3)
C3—H3	0.9300	C21—C22	1.377 (3)

C4—C5	1.363 (3)	C21—N9	1.4302 (19)
C4—H4	0.9300	C22—C23	1.386 (3)
C5—C6	1.387 (3)	C22—H22	0.9300
C5—H5	0.9300	C23—C24	1.362 (4)
C6—H6	0.9300	C23—H23	0.9300
C7—N1	1.3486 (19)	C24—C25	1.377 (4)
C7—C8	1.374 (2)	C24—H24	0.9300
C7—C9	1.479 (2)	C25—C26	1.384 (3)
C8—N3	1.351 (2)	C25—H25	0.9300
C8—C10	1.474 (2)	C26—H26	0.9300
C9—H9A	0.9600	C27—N9	1.350 (2)
C9—H9B	0.9600	C27—C28	1.372 (2)
C9—H9C	0.9600	C27—C29	1.474 (2)
C10—O1	1.2217 (19)	C28—N11	1.355 (2)
C10—N4	1.348 (2)	C28—C30	1.474 (2)
C11—O2	1.2195 (19)	C29—H29A	0.9600
C11—N5	1.353 (2)	C29—H29B	0.9600
C11—C12	1.476 (2)	C29—H29C	0.9600
C12—N6	1.357 (2)	C30—O3	1.221 (2)
C12—C13	1.374 (2)	C30—N12	1.351 (2)
C13—N8	1.3505 (19)	N1—N2	1.369 (2)
C13—C14	1.484 (2)	N2—N3	1.3003 (19)
C14—H14A	0.9600	N4—N5	1.3802 (17)
C14—H14B	0.9600	N4—H4A	0.8600
C14—H14C	0.9600	N5—H5A	0.8600
C15—C16	1.366 (3)	N6—N7	1.3019 (18)
C15—C20	1.382 (3)	N7—N8	1.368 (2)
C15—N8	1.434 (2)	N9—N10	1.365 (2)
C16—C17	1.380 (3)	N10—N11	1.2994 (18)
C16—H16	0.9300	N12—N12^{i}	1.388 (2)
C17—C18	1.368 (4)	N12—H12	0.8600
C17—H17	0.9300		

C2—C1—C6	121.10 (17)	C20—C19—H19	119.8
C2—C1—N1	118.70 (15)	C15—C20—C19	118.5 (2)
C6—C1—N1	120.19 (16)	C15—C20—H20	120.8
C1—C2—C3	118.84 (19)	C19—C20—H20	120.8
C1—C2—H2	120.6	C26—C21—C22	120.80 (17)
C3—C2—H2	120.6	C26—C21—N9	117.95 (16)
C4—C3—C2	120.5 (2)	C22—C21—N9	121.21 (16)
C4—C3—H3	119.7	C21—C22—C23	119.38 (19)
C2—C3—H3	119.7	C21—C22—H22	120.3
C5—C4—C3	120.11 (19)	C23—C22—H22	120.3
C5—C4—H4	119.9	C24—C23—C22	120.4 (2)
C3—C4—H4	119.9	C24—C23—H23	119.8
C4—C5—C6	120.2 (2)	C22—C23—H23	119.8
C4—C5—H5	119.9	C23—C24—C25	119.84 (19)
C6—C5—H5	119.9	C23—C24—H24	120.1

C1—C6—C5	119.2 (2)	C25—C24—H24	120.1
C1—C6—H6	120.4	C24—C25—C26	120.7 (2)
C5—C6—H6	120.4	C24—C25—H25	119.7
N1—C7—C8	103.20 (14)	C26—C25—H25	119.7
N1—C7—C9	124.85 (14)	C21—C26—C25	118.9 (2)
C8—C7—C9	131.95 (14)	C21—C26—H26	120.5
N3—C8—C7	109.91 (13)	C25—C26—H26	120.5
N3—C8—C10	121.97 (14)	N9—C27—C28	103.39 (14)
C7—C8—C10	128.07 (14)	N9—C27—C29	125.11 (15)
C7—C9—H9A	109.5	C28—C27—C29	131.50 (15)
C7—C9—H9B	109.5	N11—C28—C27	109.76 (13)
H9A—C9—H9B	109.5	N11—C28—C30	121.58 (15)
C7—C9—H9C	109.5	C27—C28—C30	128.64 (15)
H9A—C9—H9C	109.5	C27—C29—H29A	109.5
H9B—C9—H9C	109.5	C27—C29—H29B	109.5
O1—C10—N4	123.41 (14)	H29A—C29—H29B	109.5
O1—C10—C8	122.48 (15)	C27—C29—H29C	109.5
N4—C10—C8	114.08 (14)	H29A—C29—H29C	109.5
O2—C11—N5	123.48 (14)	H29B—C29—H29C	109.5
O2—C11—C12	122.96 (15)	O3—C30—N12	123.03 (15)
N5—C11—C12	113.53 (14)	O3—C30—C28	122.77 (16)
N6—C12—C13	109.89 (13)	N12—C30—C28	114.16 (14)
N6—C12—C11	121.82 (14)	C7—N1—N2	111.19 (12)
C13—C12—C11	128.28 (15)	C7—N1—C1	130.57 (14)
N8—C13—C12	103.27 (14)	N2—N1—C1	118.15 (13)
N8—C13—C14	125.91 (14)	N3—N2—N1	106.73 (13)
C12—C13—C14	130.79 (14)	N2—N3—C8	108.97 (14)
C13—C14—H14A	109.5	C10—N4—N5	120.00 (13)
C13—C14—H14B	109.5	C10—N4—H4A	120.0
H14A—C14—H14B	109.5	N5—N4—H4A	120.0
C13—C14—H14C	109.5	C11—N5—N4	119.44 (13)
H14A—C14—H14C	109.5	C11—N5—H5A	120.3
H14B—C14—H14C	109.5	N4—N5—H5A	120.3
C16—C15—C20	121.42 (18)	N7—N6—C12	108.70 (14)
C16—C15—N8	120.36 (16)	N6—N7—N8	106.98 (13)
C20—C15—N8	118.19 (18)	C13—N8—N7	111.16 (13)
C15—C16—C17	119.3 (2)	C13—N8—C15	130.57 (15)
C15—C16—H16	120.4	N7—N8—C15	118.25 (13)
C17—C16—H16	120.4	C27—N9—N10	111.01 (13)
C18—C17—C16	120.3 (3)	C27—N9—C21	130.64 (15)
C18—C17—H17	119.8	N10—N9—C21	118.03 (14)
C16—C17—H17	119.8	N11—N10—N9	107.05 (13)
C17—C18—C19	120.1 (2)	N10—N11—C28	108.78 (14)
C17—C18—H18	120.0	C30—N12—N12^{i}	118.92 (14)
C19—C18—H18	120.0	C30—N12—H12	120.5
C18—C19—C20	120.5 (2)	N12^{i}—N12—H12	120.5
C18—C19—H19	119.8		

C10—N4—N5—C11	−83.4 (2)	C30—N12—N12^{i}—C30^{i}	−86.4 (3)

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O1^{ii}	0.86	2.24	2.9412 (19)	139
N5—H5*A*···O2^{iii}	0.86	2.23	2.9395 (19)	140
N12—H12···O3^{iv}	0.86	2.28	3.098 (2)	158

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