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(*E*)-1-[5-Methyl-1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl]-3-(4-nitrophenyl)prop-2-en-1-one

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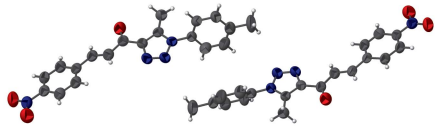
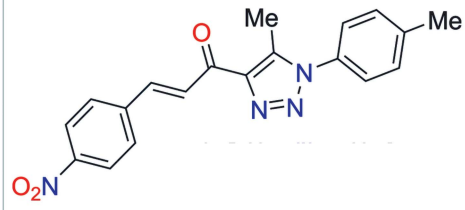
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{19}H_{16}N_4O_3$, crystallizes with two molecules (*A* and *B*) in the asymmetric unit. In molecule *A*, the dihedral angles between the triazole ring and the toluyl and nitrobenzene rings are 62.68 (16) and 10.77 (15)°, respectively. The corresponding data for molecule *B* are 68.61 (17) and 15.59 (15)°, respectively. In the crystal, the *B* molecules are linked by C—H···N hydrogen bonds to generate [001] chains. Weak C—H···π(benzene) and N—O···π(triazole) contacts are also present.

3D view



Chemical scheme



Structure description

Chalcones and their derivatives can be synthesized by Aldol or Claisen–Schmidt condensation reactions (Ahmad *et al.*, 2016; Jung *et al.*, 2017; Özdemir *et al.*, 2017; Zhuang *et al.*, 2017). As part of our studies in this area, we now describe the synthesis and structure of the title compound.

The asymmetric unit comprises two independent molecules, *A* (containing C1) and *B* (containing C20) (Fig. 1). For molecule *A*, the dihedral angles between the triazolyl and toluyl and nitrobenzene rings are 62.68 (16) and 10.77 (15)°, respectively. The corresponding data for molecule *B* are 68.61 (17) and 15.59 (15)°, respectively. In the crystal (Fig. 2), the *B* molecules are linked by C—H···N hydrogen bonds, generating [001] chains (Table 1). Weak C—H···π and N—O···π contacts (Table 1, Fig. 2) may help to consolidate the packing.

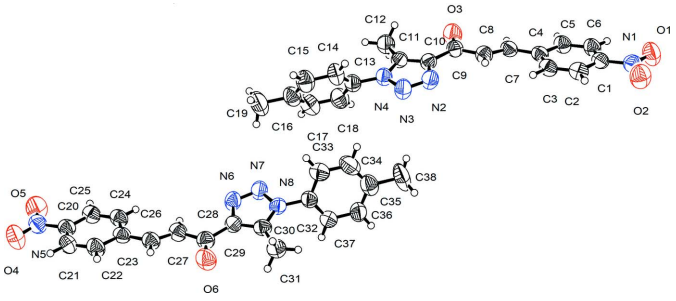


Figure 1
The molecular structure showing 50% probability ellipsoids.

Synthesis and crystallization

An equimolar mixture of 1-(1-*p*-tolyl-1*H*-1,2,3-triazol-4-yl)-ethanone and 4-nitrobenzaldehyde was reacted in aqueous ethanol (90%) containing sodium hydroxide (5%) at room temperature for 4 h. The solid obtained was collected by filtration, successively washed with water and ethanol, then dried. Crystallization of the crude product from dimethyl-formamide solution gave colourless plates (73%) of the title compound, m.p. 206–208°C.

Refinement

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

Acknowledgements

The authors extend their appreciation to the College of Applied Medical Sciences Research Centre and the Deanship of Scientific Research at King Saud University for their funding of this research.

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

*Cg*1, *Cg*4 and *Cg*6 are the centroids of the N2/N3/N4/C11/C10, N6–N8/C30/C29 and C32–C37 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C37—H37···N7^{i}	0.93	2.57	3.470 (4)	164
C36—H36···*Cg*6^{i}	0.93	3.00	3.646 (4)	128
N1—O1···*Cg*1^{ii}	1.23 (1)	3.30 (1)	3.724 (3)	101 (1)
N5—O4···*Cg*4^{iii}	1.22 (1)	3.26 (1)	3.565 (3)	94 (1)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{16}N_4O_3$
M_r	348.36
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298
a, *b*, *c* (Å)	37.0489 (16), 13.3154 (7), 6.9170 (4)
β (°)	93.771 (4)
V (Å^3)	3404.9 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.32 × 0.10 × 0.05
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.674, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	63124, 8971, 3659
R_{int}	0.068
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.699
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.076, 0.267, 1.03
No. of reflections	8971
No. of parameters	474
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), *SHELXS* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

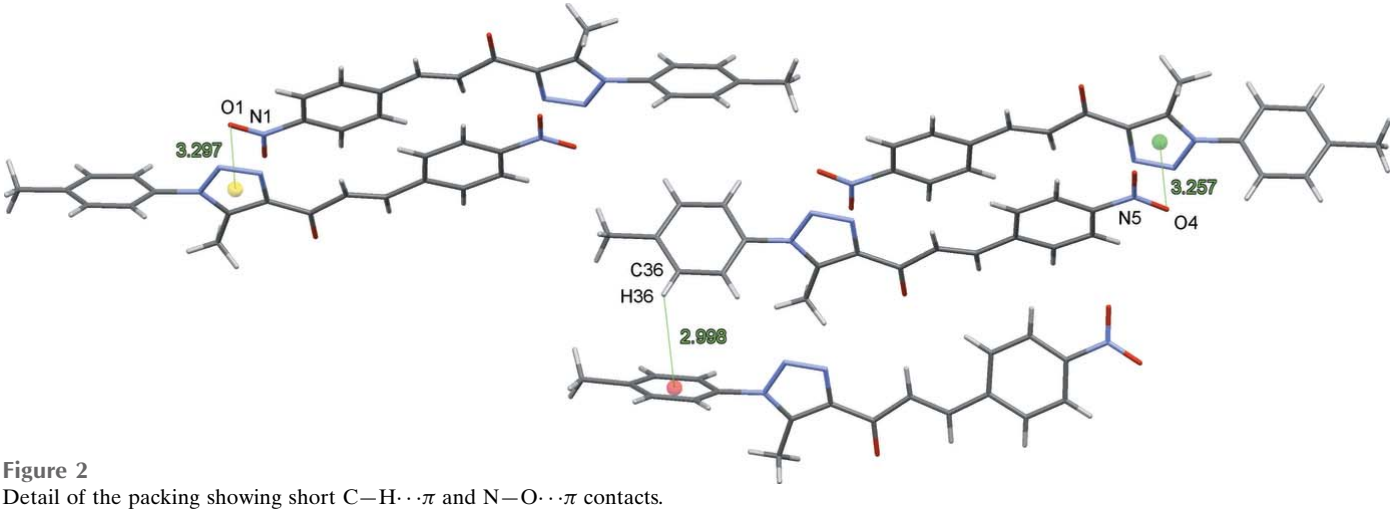

Figure 2
Detail of the packing showing short C—H···π and N—O···π contacts.

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full crystallographic data

IUCrData (2018). **3**, x180841 [https://doi.org/10.1107/S2414314618008416]

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Crystal data

$C_{19}H_{16}N_4O_3$
M_r = 348.36
Monoclinic, $P2_1/c$
a = 37.0489 (16) Å
b = 13.3154 (7) Å
c = 6.9170 (4) Å
β = 93.771 (4)°
V = 3404.9 (3) Å^3
Z = 8
$F(000)$ = 1456
D_x = 1.359 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6548 reflections
θ = 3.6–23.5°
μ = 0.10 mm^{-1}
T = 298 K
Plate, colourless
0.32 × 0.10 × 0.05 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.674, T_{max} = 1.000
63124 measured reflections
8971 independent reflections
3659 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 29.8°, θ_{min} = 0.6°
h = −49→50
k = −16→18
l = −8→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.267
S = 1.03
8971 reflections
474 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0948P)^2 + 1.2738P]$ 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}
Extinction correction: SHELXL2018 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0014 (5)

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. Non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in calculated positions and refined using a riding model. Aromatic C—H distances were set to 0.93 Å 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 Å with U(iso) set to 1.5 times the U_{eq} for the C 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	−0.07838 (7)	0.12435 (19)	−0.2371 (4)	0.0580 (7)
C2	−0.04399 (8)	0.1502 (2)	−0.2812 (5)	0.0627 (8)
H2	−0.039433	0.172105	−0.404890	0.075*
C3	−0.01634 (8)	0.1429 (2)	−0.1384 (5)	0.0599 (7)
H3	0.007096	0.159754	−0.166562	0.072*
C4	−0.02302 (7)	0.11057 (19)	0.0478 (4)	0.0543 (7)
C5	−0.05831 (7)	0.0828 (2)	0.0840 (4)	0.0631 (8)
H5	−0.063094	0.058709	0.205980	0.076*
C6	−0.08603 (8)	0.0902 (2)	−0.0567 (5)	0.0648 (8)
H6	−0.109505	0.072585	−0.030726	0.078*
C7	0.00480 (7)	0.1046 (2)	0.2058 (4)	0.0592 (7)
H7	−0.002538	0.078724	0.321835	0.071*
C8	0.03925 (8)	0.1312 (2)	0.2057 (5)	0.0619 (8)
H8	0.047871	0.158574	0.093852	0.074*
C9	0.06411 (8)	0.1186 (2)	0.3780 (5)	0.0603 (7)
C10	0.10290 (7)	0.1286 (2)	0.3535 (4)	0.0560 (7)
C11	0.13136 (7)	0.1187 (2)	0.4903 (4)	0.0553 (7)
C12	0.13269 (8)	0.0982 (3)	0.7006 (4)	0.0721 (9)
H12A	0.129704	0.027512	0.721556	0.108*
H12B	0.113607	0.134274	0.757428	0.108*
H12C	0.155609	0.119531	0.759303	0.108*
C13	0.19821 (8)	0.1305 (2)	0.4518 (4)	0.0608 (7)
C14	0.21867 (8)	0.2157 (3)	0.4340 (5)	0.0753 (9)
H14	0.208141	0.274356	0.383623	0.090*
C15	0.25505 (9)	0.2132 (3)	0.4920 (5)	0.0826 (10)
H15	0.268888	0.270852	0.479493	0.099*
C16	0.27134 (9)	0.1279 (3)	0.5677 (5)	0.0765 (9)
C17	0.25024 (10)	0.0440 (3)	0.5858 (5)	0.0898 (11)
H17	0.260667	−0.014127	0.638841	0.108*
C18	0.21388 (9)	0.0441 (3)	0.5269 (5)	0.0788 (9)
H18	0.200120	−0.013821	0.537950	0.095*
C19	0.31105 (9)	0.1268 (3)	0.6318 (6)	0.1083 (14)
H19A	0.322354	0.186336	0.586151	0.162*
H19B	0.322231	0.068656	0.579273	0.162*

H19C	0.313852	0.124572	0.770678	0.162*
C20	0.58057 (8)	−0.1266 (2)	0.7190 (5)	0.0632 (8)
C21	0.58744 (8)	−0.0966 (2)	0.5356 (5)	0.0711 (9)
H21	0.610895	−0.081986	0.504159	0.085*
C22	0.55883 (8)	−0.0886 (2)	0.3986 (5)	0.0718 (9)
H22	0.563061	−0.066482	0.274590	0.086*
C23	0.52374 (8)	−0.1128 (2)	0.4423 (5)	0.0603 (7)
C24	0.51790 (8)	−0.1418 (2)	0.6319 (5)	0.0653 (8)
H24	0.494571	−0.156823	0.664967	0.078*
C25	0.54634 (8)	−0.1486 (2)	0.7709 (5)	0.0657 (8)
H25	0.542365	−0.167648	0.897098	0.079*
C26	0.49517 (8)	−0.1071 (2)	0.2878 (5)	0.0658 (8)
H26	0.502228	−0.084686	0.168661	0.079*
C27	0.46064 (8)	−0.1294 (2)	0.2946 (5)	0.0675 (8)
H27	0.452087	−0.151649	0.410576	0.081*
C28	0.43530 (8)	−0.1200 (2)	0.1224 (5)	0.0645 (8)
C29	0.39649 (8)	−0.1240 (2)	0.1530 (4)	0.0591 (7)
C30	0.36728 (8)	−0.1201 (2)	0.0187 (4)	0.0583 (7)
C31	0.36487 (9)	−0.1119 (3)	−0.1951 (4)	0.0731 (9)
H31A	0.341635	−0.135380	−0.245605	0.110*
H31B	0.383516	−0.151866	−0.246773	0.110*
H31C	0.367886	−0.042954	−0.231519	0.110*
C32	0.30061 (8)	−0.1231 (2)	0.0704 (4)	0.0613 (7)
C33	0.27922 (9)	−0.0428 (3)	0.1153 (5)	0.0832 (10)
H33	0.289304	0.013852	0.176028	0.100*
C34	0.24234 (10)	−0.0485 (3)	0.0680 (6)	0.0915 (11)
H34	0.227794	0.005537	0.097475	0.110*
C35	0.22651 (9)	−0.1313 (3)	−0.0210 (5)	0.0820 (10)
C36	0.24885 (8)	−0.2099 (3)	−0.0643 (5)	0.0794 (10)
H36	0.238849	−0.266349	−0.126179	0.095*
C37	0.28570 (8)	−0.2070 (3)	−0.0181 (5)	0.0717 (9)
H37	0.300229	−0.261252	−0.046600	0.086*
C38	0.18607 (9)	−0.1370 (4)	−0.0680 (6)	0.1171 (16)
H38A	0.176022	−0.189193	0.007869	0.176*
H38B	0.181355	−0.151663	−0.203171	0.176*
H38C	0.175199	−0.073923	−0.038342	0.176*
N1	−0.10784 (8)	0.13323 (19)	−0.3873 (4)	0.0706 (7)
N2	0.11600 (7)	0.1475 (2)	0.1767 (4)	0.0681 (7)
N3	0.15105 (7)	0.1491 (2)	0.1965 (4)	0.0724 (7)
N4	0.16083 (6)	0.13206 (18)	0.3880 (3)	0.0604 (6)
N5	0.61118 (8)	−0.13453 (19)	0.8654 (5)	0.0738 (7)
N6	0.38406 (7)	−0.12831 (19)	0.3349 (4)	0.0689 (7)
N7	0.34928 (7)	−0.1266 (2)	0.3210 (4)	0.0726 (7)
N8	0.33869 (6)	−0.12202 (18)	0.1281 (3)	0.0606 (6)
O1	−0.13863 (6)	0.1115 (2)	−0.3461 (4)	0.0946 (8)
O2	−0.10091 (7)	0.1614 (2)	−0.5489 (4)	0.0976 (8)
O3	0.05331 (6)	0.0976 (2)	0.5370 (3)	0.0866 (7)
O4	0.64161 (7)	−0.1192 (2)	0.8154 (4)	0.1034 (9)

O5	0.60489 (7)	−0.1547 (2)	1.0319 (4)	0.1060 (9)
O6	0.44557 (6)	−0.1070 (2)	−0.0403 (4)	0.0931 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0532 (17)	0.0548 (16)	0.0664 (19)	0.0035 (12)	0.0071 (14)	−0.0021 (14)
C2	0.0662 (19)	0.0568 (17)	0.067 (2)	−0.0019 (13)	0.0151 (15)	0.0063 (14)
C3	0.0507 (16)	0.0559 (17)	0.075 (2)	−0.0062 (12)	0.0175 (15)	0.0027 (14)
C4	0.0482 (15)	0.0498 (15)	0.0659 (18)	−0.0015 (11)	0.0124 (13)	−0.0047 (13)
C5	0.0530 (17)	0.0751 (19)	0.0626 (19)	−0.0030 (14)	0.0147 (14)	0.0042 (15)
C6	0.0482 (16)	0.077 (2)	0.070 (2)	−0.0022 (13)	0.0143 (15)	0.0023 (16)
C7	0.0508 (16)	0.0584 (17)	0.0694 (19)	−0.0001 (12)	0.0114 (14)	−0.0065 (14)
C8	0.0569 (18)	0.0591 (18)	0.070 (2)	−0.0041 (12)	0.0063 (14)	0.0004 (14)
C9	0.0517 (17)	0.0634 (18)	0.067 (2)	−0.0047 (12)	0.0086 (14)	−0.0042 (14)
C10	0.0544 (17)	0.0588 (17)	0.0551 (17)	−0.0052 (12)	0.0055 (13)	−0.0021 (13)
C11	0.0522 (16)	0.0640 (17)	0.0509 (16)	−0.0056 (12)	0.0111 (13)	−0.0025 (13)
C12	0.0648 (19)	0.094 (2)	0.0578 (19)	−0.0033 (16)	0.0097 (15)	0.0030 (16)
C13	0.0523 (17)	0.082 (2)	0.0484 (16)	−0.0002 (14)	0.0081 (13)	−0.0001 (14)
C14	0.0531 (18)	0.091 (2)	0.081 (2)	−0.0015 (16)	−0.0004 (15)	0.0130 (18)
C15	0.065 (2)	0.098 (3)	0.086 (2)	−0.0084 (18)	0.0080 (17)	0.012 (2)
C16	0.0585 (19)	0.108 (3)	0.064 (2)	0.0062 (18)	0.0111 (15)	0.0039 (19)
C17	0.072 (2)	0.105 (3)	0.094 (3)	0.019 (2)	0.0116 (19)	0.018 (2)
C18	0.067 (2)	0.082 (2)	0.088 (2)	−0.0019 (17)	0.0091 (17)	0.0082 (19)
C19	0.059 (2)	0.152 (4)	0.113 (3)	0.011 (2)	0.004 (2)	0.006 (3)
C20	0.0609 (19)	0.0534 (17)	0.076 (2)	0.0014 (13)	0.0101 (16)	−0.0024 (15)
C21	0.0543 (18)	0.083 (2)	0.078 (2)	−0.0059 (14)	0.0162 (16)	−0.0006 (17)
C22	0.0600 (19)	0.083 (2)	0.074 (2)	−0.0078 (15)	0.0194 (16)	0.0048 (17)
C23	0.0596 (18)	0.0510 (16)	0.072 (2)	0.0007 (12)	0.0143 (15)	−0.0025 (14)
C24	0.0580 (18)	0.0580 (18)	0.082 (2)	−0.0059 (13)	0.0202 (16)	0.0014 (15)
C25	0.0653 (19)	0.0604 (18)	0.073 (2)	−0.0025 (14)	0.0156 (16)	0.0068 (15)
C26	0.0598 (19)	0.0648 (18)	0.074 (2)	−0.0031 (13)	0.0155 (16)	−0.0007 (15)
C27	0.0639 (19)	0.0631 (19)	0.076 (2)	−0.0044 (13)	0.0108 (16)	0.0025 (15)
C28	0.0620 (19)	0.0643 (18)	0.068 (2)	−0.0047 (13)	0.0123 (16)	−0.0009 (15)
C29	0.0585 (18)	0.0630 (18)	0.0565 (18)	−0.0063 (13)	0.0080 (14)	−0.0006 (13)
C30	0.0619 (18)	0.0612 (17)	0.0533 (17)	−0.0027 (13)	0.0146 (14)	0.0002 (13)
C31	0.072 (2)	0.095 (2)	0.0527 (18)	0.0003 (16)	0.0104 (15)	0.0041 (16)
C32	0.0520 (17)	0.081 (2)	0.0513 (17)	0.0014 (14)	0.0087 (13)	−0.0022 (15)
C33	0.079 (2)	0.093 (2)	0.079 (2)	0.0093 (18)	0.0122 (18)	−0.0109 (19)
C34	0.076 (2)	0.113 (3)	0.087 (3)	0.029 (2)	0.0158 (19)	0.001 (2)
C35	0.062 (2)	0.122 (3)	0.063 (2)	0.006 (2)	0.0097 (16)	0.014 (2)
C36	0.0568 (19)	0.111 (3)	0.070 (2)	−0.0038 (18)	0.0024 (15)	−0.0100 (19)
C37	0.0595 (19)	0.087 (2)	0.069 (2)	0.0032 (16)	0.0077 (15)	−0.0144 (17)
C38	0.049 (2)	0.189 (5)	0.114 (3)	0.009 (2)	0.004 (2)	0.034 (3)
N1	0.0702 (19)	0.0667 (17)	0.075 (2)	0.0048 (12)	0.0063 (15)	−0.0023 (14)
N2	0.0590 (16)	0.0903 (18)	0.0553 (16)	−0.0104 (12)	0.0056 (12)	0.0003 (13)
N3	0.0589 (16)	0.105 (2)	0.0532 (16)	−0.0093 (13)	0.0056 (12)	0.0033 (14)
N4	0.0528 (14)	0.0773 (16)	0.0516 (14)	−0.0035 (11)	0.0064 (11)	0.0016 (12)

N5	0.0654 (18)	0.0686 (17)	0.088 (2)	0.0019 (12)	0.0051 (16)	0.0007 (15)
N6	0.0574 (16)	0.0926 (19)	0.0569 (16)	−0.0143 (12)	0.0045 (12)	−0.0005 (13)
N7	0.0579 (16)	0.109 (2)	0.0514 (15)	−0.0133 (13)	0.0076 (12)	−0.0052 (14)
N8	0.0597 (15)	0.0761 (16)	0.0465 (14)	−0.0053 (11)	0.0082 (11)	−0.0032 (11)
O1	0.0585 (15)	0.124 (2)	0.1007 (19)	−0.0007 (13)	−0.0004 (13)	0.0072 (15)
O2	0.0954 (19)	0.121 (2)	0.0752 (18)	0.0013 (15)	0.0009 (14)	0.0185 (15)
O3	0.0658 (14)	0.127 (2)	0.0683 (15)	−0.0105 (12)	0.0155 (11)	0.0042 (14)
O4	0.0617 (16)	0.134 (2)	0.114 (2)	−0.0016 (13)	0.0062 (14)	0.0149 (17)
O5	0.0969 (19)	0.138 (2)	0.083 (2)	0.0019 (16)	0.0039 (15)	0.0209 (17)
O6	0.0722 (15)	0.137 (2)	0.0726 (16)	−0.0047 (13)	0.0210 (12)	0.0044 (14)

Geometric parameters (Å, º)

C1—C2	1.373 (4)	C21—H21	0.9300
C1—C6	1.375 (4)	C22—C23	1.392 (4)
C1—N1	1.462 (4)	C22—H22	0.9300
C2—C3	1.379 (4)	C23—C24	1.398 (4)
C2—H2	0.9300	C23—C26	1.456 (4)
C3—C4	1.395 (4)	C24—C25	1.382 (4)
C3—H3	0.9300	C24—H24	0.9300
C4—C5	1.397 (4)	C25—H25	0.9300
C4—C7	1.454 (4)	C26—C27	1.317 (4)
C5—C6	1.372 (4)	C26—H26	0.9300
C5—H5	0.9300	C27—C28	1.473 (5)
C6—H6	0.9300	C27—H27	0.9300
C7—C8	1.325 (4)	C28—O6	1.223 (4)
C7—H7	0.9300	C28—C29	1.468 (4)
C8—C9	1.467 (4)	C29—N6	1.369 (4)
C8—H8	0.9300	C29—C30	1.380 (4)
C9—O3	1.228 (3)	C30—N8	1.342 (3)
C9—C10	1.464 (4)	C30—C31	1.480 (4)
C10—N2	1.368 (3)	C31—H31A	0.9600
C10—C11	1.376 (4)	C31—H31B	0.9600
C11—N4	1.351 (3)	C31—H31C	0.9600
C11—C12	1.478 (4)	C32—C37	1.372 (4)
C12—H12A	0.9600	C32—C33	1.378 (4)
C12—H12B	0.9600	C32—N8	1.441 (4)
C12—H12C	0.9600	C33—C34	1.386 (5)
C13—C18	1.375 (4)	C33—H33	0.9300
C13—C14	1.375 (4)	C34—C35	1.375 (5)
C13—N4	1.426 (4)	C34—H34	0.9300
C14—C15	1.381 (4)	C35—C36	1.379 (5)
C14—H14	0.9300	C35—C38	1.514 (5)
C15—C16	1.375 (5)	C36—C37	1.382 (4)
C15—H15	0.9300	C36—H36	0.9300
C16—C17	1.373 (5)	C37—H37	0.9300
C16—C19	1.509 (5)	C38—H38A	0.9600
C17—C18	1.381 (5)	C38—H38B	0.9600

C17—H17	0.9300	C38—H38C	0.9600
C18—H18	0.9300	N1—O2	1.222 (3)
C19—H19A	0.9600	N1—O1	1.229 (3)
C19—H19B	0.9600	N2—N3	1.297 (3)
C19—H19C	0.9600	N3—N4	1.369 (3)
C20—C21	1.370 (4)	N5—O4	1.218 (3)
C20—C25	1.372 (4)	N5—O5	1.220 (3)
C20—N5	1.473 (4)	N6—N7	1.286 (3)
C21—C22	1.379 (4)	N7—N8	1.367 (3)
C2—C1—C6	122.3 (3)	C23—C22—H22	119.3
C2—C1—N1	118.8 (3)	C22—C23—C24	118.2 (3)
C6—C1—N1	118.9 (3)	C22—C23—C26	118.2 (3)
C1—C2—C3	118.7 (3)	C24—C23—C26	123.6 (3)
C1—C2—H2	120.7	C25—C24—C23	120.8 (3)
C3—C2—H2	120.7	C25—C24—H24	119.6
C2—C3—C4	121.0 (3)	C23—C24—H24	119.6
C2—C3—H3	119.5	C20—C25—C24	118.7 (3)
C4—C3—H3	119.5	C20—C25—H25	120.7
C3—C4—C5	118.2 (3)	C24—C25—H25	120.7
C3—C4—C7	123.4 (2)	C27—C26—C23	128.5 (3)
C5—C4—C7	118.4 (3)	C27—C26—H26	115.7
C6—C5—C4	121.3 (3)	C23—C26—H26	115.7
C6—C5—H5	119.4	C26—C27—C28	121.4 (3)
C4—C5—H5	119.4	C26—C27—H27	119.3
C5—C6—C1	118.6 (3)	C28—C27—H27	119.3
C5—C6—H6	120.7	O6—C28—C29	120.3 (3)
C1—C6—H6	120.7	O6—C28—C27	122.4 (3)
C8—C7—C4	128.3 (3)	C29—C28—C27	117.3 (3)
C8—C7—H7	115.9	N6—C29—C30	108.9 (2)
C4—C7—H7	115.9	N6—C29—C28	121.7 (3)
C7—C8—C9	121.5 (3)	C30—C29—C28	129.3 (3)
C7—C8—H8	119.3	N8—C30—C29	103.5 (2)
C9—C8—H8	119.3	N8—C30—C31	124.5 (3)
O3—C9—C10	120.3 (3)	C29—C30—C31	132.0 (3)
O3—C9—C8	122.0 (3)	C30—C31—H31A	109.5
C10—C9—C8	117.6 (3)	C30—C31—H31B	109.5
N2—C10—C11	109.3 (2)	H31A—C31—H31B	109.5
N2—C10—C9	121.9 (3)	C30—C31—H31C	109.5
C11—C10—C9	128.7 (3)	H31A—C31—H31C	109.5
N4—C11—C10	103.7 (2)	H31B—C31—H31C	109.5
N4—C11—C12	124.3 (3)	C37—C32—C33	120.8 (3)
C10—C11—C12	132.0 (2)	C37—C32—N8	119.3 (3)
C11—C12—H12A	109.5	C33—C32—N8	119.8 (3)
C11—C12—H12B	109.5	C32—C33—C34	118.5 (3)
H12A—C12—H12B	109.5	C32—C33—H33	120.8
C11—C12—H12C	109.5	C34—C33—H33	120.8
H12A—C12—H12C	109.5	C35—C34—C33	122.3 (3)

H12B—C12—H12C	109.5	C35—C34—H34	118.8
C18—C13—C14	120.2 (3)	C33—C34—H34	118.8
C18—C13—N4	120.4 (3)	C34—C35—C36	117.4 (3)
C14—C13—N4	119.4 (3)	C34—C35—C38	121.6 (4)
C13—C14—C15	119.2 (3)	C36—C35—C38	121.0 (4)
C13—C14—H14	120.4	C35—C36—C37	121.8 (3)
C15—C14—H14	120.4	C35—C36—H36	119.1
C16—C15—C14	121.8 (3)	C37—C36—H36	119.1
C16—C15—H15	119.1	C32—C37—C36	119.2 (3)
C14—C15—H15	119.1	C32—C37—H37	120.4
C17—C16—C15	117.9 (3)	C36—C37—H37	120.4
C17—C16—C19	121.0 (3)	C35—C38—H38A	109.5
C15—C16—C19	121.0 (3)	C35—C38—H38B	109.5
C16—C17—C18	121.5 (3)	H38A—C38—H38B	109.5
C16—C17—H17	119.2	C35—C38—H38C	109.5
C18—C17—H17	119.2	H38A—C38—H38C	109.5
C13—C18—C17	119.4 (3)	H38B—C38—H38C	109.5
C13—C18—H18	120.3	O2—N1—O1	122.6 (3)
C17—C18—H18	120.3	O2—N1—C1	118.9 (3)
C16—C19—H19A	109.5	O1—N1—C1	118.5 (3)
C16—C19—H19B	109.5	N3—N2—C10	108.7 (2)
H19A—C19—H19B	109.5	N2—N3—N4	107.4 (2)
C16—C19—H19C	109.5	C11—N4—N3	110.9 (2)
H19A—C19—H19C	109.5	C11—N4—C13	129.7 (3)
H19B—C19—H19C	109.5	N3—N4—C13	119.4 (2)
C21—C20—C25	122.4 (3)	O4—N5—O5	122.9 (3)
C21—C20—N5	118.4 (3)	O4—N5—C20	118.5 (3)
C25—C20—N5	119.2 (3)	O5—N5—C20	118.6 (3)
C20—C21—C22	118.5 (3)	N7—N6—C29	109.0 (2)
C20—C21—H21	120.7	N6—N7—N8	107.2 (2)
C22—C21—H21	120.7	C30—N8—N7	111.4 (2)
C21—C22—C23	121.3 (3)	C30—N8—C32	129.7 (3)
C21—C22—H22	119.3	N7—N8—C32	118.9 (2)

Hydrogen-bond geometry (Å, º)

Cg1, Cg4 and Cg6 are the centroids of the N2/N3/N4/C11/C10, N6–N8/C30/C29 and C32–C37 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C37—H37···N7^{i}	0.93	2.57	3.470 (4)	164
C36—H36···*Cg*6^{i}	0.93	3.00	3.646 (4)	128
N1—O1···*Cg*1^{ii}	1.23 (1)	3.30 (1)	3.724 (3)	101 (1)
N5—O4···*Cg*4^{iii}	1.22 (1)	3.26 (1)	3.565 (3)	94 (1)

Symmetry codes: (i) x, $-y-1/2$, $z-1/2$; (ii) $-x$, $-y$, $-z$; (iii) $-x+1$, $-y$, $-z+1$.