5-(2-Methylfuran-3-yl)-N-phenyl-1,3,4-oxadiazol-2-amine

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In the title compound, $C_{13}H_{11}N_3O_2$, the furan ring is disordered over two orientations, with occupancies of 0.902 (2) and 0.098 (2). The dihedral angles between the central oxadiazole ring and the pendant phenyl ring and the furan ring (major disorder component) are 10.12 (11) and 1.76 (15)°, respectively. A short intramolecular C—H···O contact generates an $S(6)$ ring. In the crystal, inversion dimers linked by pairs of N—H···N hydrogen bonds generate $R_2^2(8)$ loops. The dimers are linked by C—H···π and π–π interactions [range of centroid–centroid distances = 3.301 (7)–3.689 (1) Å], generating a three-dimensional network.

3D view

Chemical scheme

Structure description

The coordination chemistry of nitrogen–oxygen containing heterocyclic ligands such as 1,3,4-oxadiazoles and their derivatives containing the HNCO moiety is an emerging and rapidly developing area of research (Wang *et al.*, 2007; Foroumadi *et al.*, 2001; Bharty *et al.*, 2012). 1,3,4-Oxadiazole derivatives have also been the subject of extensive study in the recent years because of their diverse biological activities (Luo *et al.*, 2016; Aboraia *et al.*, 2006; El-Emam *et al.*, 2004; Bharty *et al.*, 2015). These molecules can act as spacers in coordination compounds, resulting in intermolecular cooperative interactions (Du & Zhao, 2004). In the presence of a base, the cyclization of acyldithiocarbazate esters to the corresponding 1,3,4-oxadiazole is reported (Foks *et al.*, 2002). Several other methods are available for the synthesis of oxadiazoles from acyclic precursors. These include oxidative cyclization of acylhydrazones (Jedlovská & Leško, 1994) and acylthiosemicarbazides (Omar *et al.*, 1996, Paswan *et al.*, 2015). It is reported that in the presence of a strong acid,
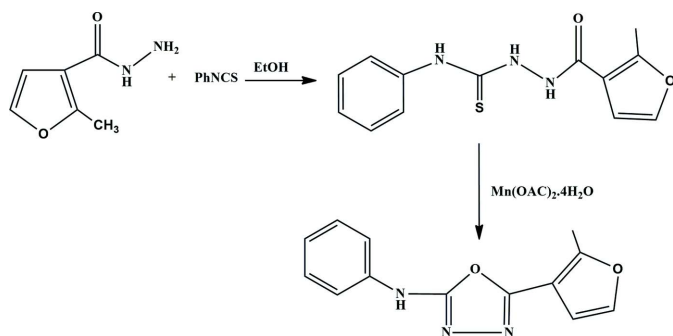
Figure 1
A reaction scheme showing the synthesis of the title compound. For clarity in this and subsequent Figures, only the major disorder component of the furan ring is shown.

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

$Cg3$, $Cg2$ are the centroids of the benzene (C1–C6) and furan (O2/C9–C12) rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$N\cdots$N2^{i}	0.92 (2)	1.97 (2)	2.885 (2)	171 (2)
C2—H2$A\cdots$O1	0.95	2.31	2.930 (2)	122
C13—H13$A\cdots$O1	0.98	2.46	3.151 (3)	127
C13A—H13$D\cdots$N3	0.98	2.65	3.41 (3)	134
C5—H5$A\cdots Cg3^{ii}$	0.95	2.89	3.655 (4)	138
C13A—H13$F\cdots Cg2^{iii}$	0.98	2.80	3.612 (8)	141

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

an *N*-acylhydrazine carbodithioate is converted to a thiadiazole whereas in the presence of weak acid or base or on complexation they can be cyclized to the corresponding oxadiazole (Reid & Heindel, 1976; Jasinski *et al.*, 2011). Previously, we have reported 1,3,4-thiadiazoles that were prepared by the reaction of a substituted thiosemicarbazide with manganese(II) nitrate, in which the substituted thiosemicarbazide cyclized to the corresponding thiadiazole *via* loss of H_2O (Dani *et al.*, 2014). However, in the present case, the substituted thiosemicarbazide is cyclized to (2-methyl)-5-furan-2-yl-[1,3,4]-oxadiazole-2-yl)phenylamine in the presence of manganese(II) acetate in this case with loss of H_2S (Fig. 1). Thus, the Mn^{II} acetate behaves here as a weak acid.

In the title compound (Fig. 2), the mean plane of the central oxadiazole ring (O1/C7/N2/N3/C8) subtends dihedral angles of 10.12 (11) and 1.76 (15)° with the furan (O2/C12/C9/C10/C11) and phenyl rings (C1–C6), respectively. The furan and phenyl rings are inclined to one another at an angle of 9.92 (14)°. Intramolecular C2—H2$A\cdots$O1 and C13—H13$A\cdots$O1 hydrogen bonds generate $S(6)$ rings, contributing to the planarity of the whole molecule. The C—N bond lengths [N2—C7 1.2947 (19) and N3—C8 1.270 (2) Å] are similar to the standard C=N distance of 1.28 Å. The C—O and C—N distances found within the oxadiazole ring are intermediate between single and double bonds, suggesting considerable delocalization in this ring. Deviation of the bond angles from
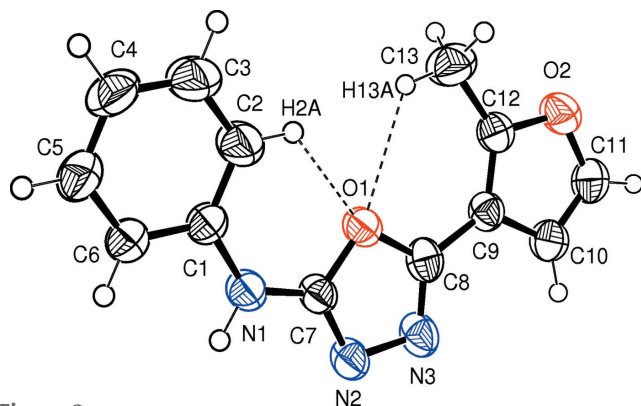
120° in the oxadiazole ring is a common feature in five-membered rings.

In the crystal, pairs of intermolecular N—H$\cdots$N hydrogen bonds between the oxadiazole ring and the amine group form dimers with an $R_2^2(8)$ ring motif (Fig. 3, Table 1). Molecules are further linked by two C—H$\cdots\pi$ interactions (Fig. 4 and Table 1) involving the (O2/C9–C12) and (C1–C6) rings. In addition, weak π–π stacking interactions [$Cg1\cdots Cg1(-x, -y, 1-z) = 3.301$ (7) Å; $Cg1\cdots Cg2(x, -1+y, z) = 3.612$ (5) Å; $Cg2\cdots Cg2$ (1/2 − x, 1/2 − y, 1 − z) = 3.689 (1) Å; $Cg1$, $Cg2$ and $Cg3$ are the centroids of the O1/C7–C8/N2–N3, O2/C9–C12 and C1–C6 rings respectively] are also present and influence the crystal packing (Fig. 5). These contacts lead to a three-dimensional structure.

Synthesis and crystallization

A mixture of 2-methyl furan-3-carboxylic acid hydrazide (1.40 g, 10.0 mmol) and phenyl isothiocyanate (1.2 ml, 10.0 mmol) in absolute ethanol (20.0 ml) was refluxed for 2 h. The solid 4-phenyl-1-(2-methyl-3-furan) thiosemicarbazide obtained upon cooling was filtered off and washed with water and ether (50:50 *v/v*). A mixture of a methanolic solution of 4-phenyl-1-(2-methyl-3-furan)thiosemicarbazide (0.275 g,

Figure 2
The molecular structure of the title compound, showing 50% probability displacement ellipsoids. Hydrogen bonds are drawn as dashed lines.
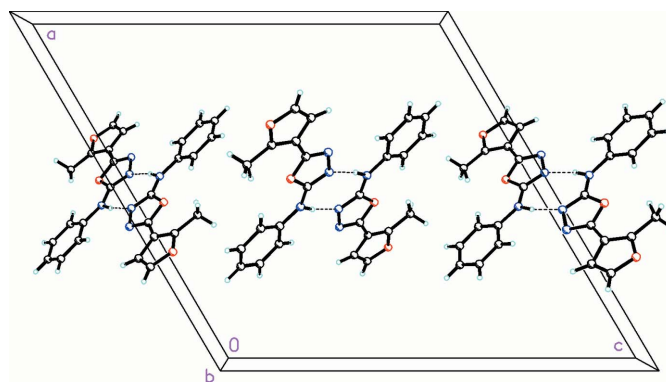

Figure 3
The crystal packing of the title compound, viewed along the *b* axis. Dashed lines indicate weak intermolecular N—H$\cdots$N hydrogen bonding between the oxadiazole ring and the amine group, forming dimers with an $R_2^2(8)$ ring motif.
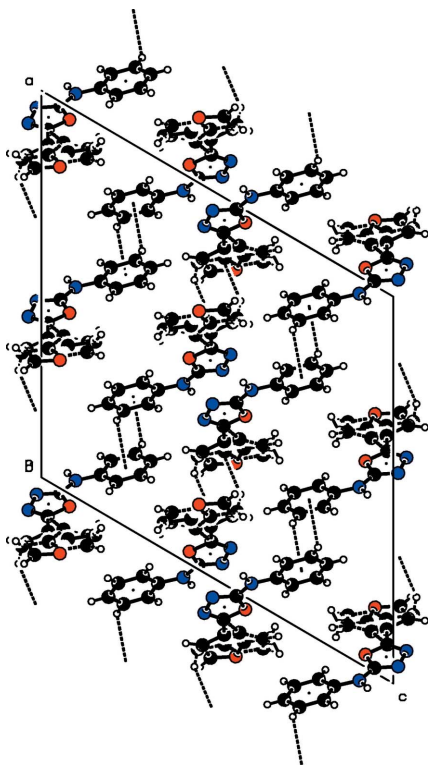
Figure 4
A view of the packing along the *b* axis, showing the C—H···π contacts.

1.00 mmol) and Mn(OAc)$_2$·4H$_2$O (0.251 g, 1.00 mmol) was stirred for 2 h. The clear orange-red solution obtained was filtered off and kept for crystallization, pale orange–red crystals of title compound suitable for X-ray analyses were obtained after eight days (Fig. 1). Yield: 60%. m.p. 205°C. Analysis: found. C, 64.35; H, 4.30; N, 17.55%. Calculated for C$_{13}$H$_{11}$N$_3$O$_2$ (241.25): C, 64.71; H, 4.59; N, 17.41%. IR (KBr, cm^{-1}): ν(N—H) 3244; ν(C=N) 1601; ν(N—N) 1061 *s*. ^{1}H NMR (DMSO-*d$_6$*), δ [p.p.m.] = 10.05 (*s*,1*H*, NH), 7.52–7.13 (*m*, 3H, furan), 7.42–6.90 (*m*, 5H, phenyl), 2.46 (*s*, 3H, CH$_3$). ^{13}C NMR (DMSO-*d$_6$*): δ [p.p.m.] = 163.2 (C7), 157.5 (C8); 139.7
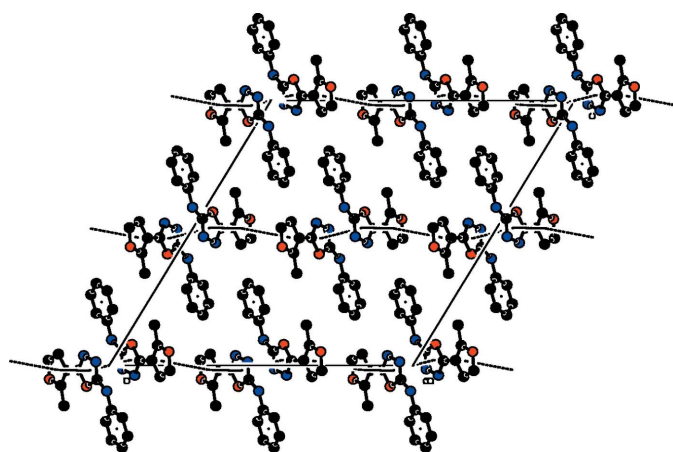

Figure 5
π–π contacts for the title compound.

Table 2
Experimental details.

Crystal data	
Chemical formula	C$_{13}$H$_{11}$N$_3$O$_2$
M_r	241.25
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	173
a, *b*, *c* (Å)	20.8964 (16), 5.9156 (3), 21.9821 (17)
β (°)	120.415 (10)
V (Å^3)	2343.4 (3)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.10
Crystal size (mm)	0.39 × 0.17 × 0.15
Data collection	
Diffractometer	Agilent Xcalibur Eos Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.814, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8528, 3895, 2403
R_{int}	0.021
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.760
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.167, 1.03
No. of reflections	3895
No. of parameters	188
No. of restraints	51
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, −0.19

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXT* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b) and *SHELXTL* (Sheldrick, 2008).

(C12), 128.4 (C11), 126.5 (C9), 125.5 (C10) (furan C); 110.6–141.1 (phenyl C), 13.8 (C13).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All atoms of the furan ring are disordered over two positions with occupancies that refine to 0.902 (2) and 0.098 (2).

Acknowledgements

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full crystallographic data

5-(2-Methylfuran-3-yl)-*N*-phenyl-1,3,4-oxadiazol-2-amine

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5-(2-Methylfuran-3-yl)-*N*-phenyl-1,3,4-oxadiazol-2-amine

Crystal data

$C_{13}H_{11}N_3O_2$	$F(000) = 1008$
$M_r = 241.25$	$D_x = 1.368$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 20.8964$ (16) Å	Cell parameters from 1741 reflections
$b = 5.9156$ (3) Å	$\theta = 4.4$–31.5°
$c = 21.9821$ (17) Å	$\mu = 0.10$ mm^{-1}
$\beta = 120.415$ (10)°	$T = 173$ K
$V = 2343.4$ (3) Å^3	Prismatic, pale orange-red
$Z = 8$	$0.39 \times 0.17 \times 0.15$ mm

Data collection

Agilent Xcalibur Eos Gemini diffractometer	8528 measured reflections
	3895 independent reflections
Radiation source: Enhance (Mo) X-ray Source	2403 reflections with $I > 2\sigma(I)$
Detector resolution: 16.0416 pixels mm^{-1}	$R_{int} = 0.021$
ω scans	$\theta_{max} = 32.7°$, $\theta_{min} = 3.6°$
Absorption correction: multi-scan	$h = -30 \rightarrow 30$
(CrysAlis PRO; Agilent, 2014)	$k = -8 \rightarrow 8$
$T_{min} = 0.814$, $T_{max} = 1.000$	$l = -33 \rightarrow 32$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent
$R[F^2 > 2\sigma(F^2)] = 0.057$	and constrained refinement
$wR(F^2) = 0.167$	$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2 + 0.7747P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
3895 reflections	$(\Delta/\sigma)_{max} < 0.001$
188 parameters	$\Delta\rho_{max} = 0.21$ e Å^{-3}
51 restraints	$\Delta\rho_{min} = -0.19$ 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.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.53261 (6)	0.43941 (18)	0.42073 (5)	0.0470 (3)	
N1	0.45640 (7)	0.1226 (2)	0.40325 (7)	0.0506 (3)	
H1N	0.4489 (10)	0.005 (3)	0.4262 (9)	0.057 (5)*	
N2	0.55136 (7)	0.2429 (2)	0.51379 (6)	0.0484 (3)	
N3	0.60380 (7)	0.4184 (2)	0.53713 (7)	0.0514 (3)	
C1	0.40324 (8)	0.1415 (3)	0.33125 (7)	0.0441 (3)	
C2	0.39829 (11)	0.3187 (3)	0.28835 (9)	0.0670 (5)	
H2A	0.4326	0.4404	0.3069	0.080*	
C3	0.34293 (12)	0.3180 (4)	0.21804 (10)	0.0761 (6)	
H3A	0.3399	0.4398	0.1885	0.091*	
C4	0.29263 (10)	0.1458 (4)	0.19026 (9)	0.0652 (5)	
H4A	0.2550	0.1474	0.1419	0.078*	
C5	0.29707 (10)	−0.0287 (4)	0.23293 (9)	0.0629 (5)	
H5A	0.2619	−0.1482	0.2142	0.075*	
C6	0.35219 (9)	−0.0330 (3)	0.30314 (8)	0.0545 (4)	
H6A	0.3551	−0.1560	0.3322	0.065*	
C7	0.51143 (8)	0.2623 (3)	0.44590 (7)	0.0424 (3)	
C8	0.59135 (8)	0.5285 (3)	0.48257 (8)	0.0465 (4)	
O2	0.66884 (14)	1.0275 (4)	0.44789 (13)	0.0586 (6)	0.902 (2)
C9	0.63019 (9)	0.7286 (3)	0.48103 (9)	0.0427 (4)	0.902 (2)
C10	0.68975 (12)	0.8339 (4)	0.54232 (11)	0.0531 (5)	0.902 (2)
H10A	0.7102	0.7862	0.5899	0.064*	0.902 (2)
C11	0.71062 (11)	1.0098 (4)	0.51977 (10)	0.0595 (5)	0.902 (2)
H11A	0.7494	1.1106	0.5494	0.071*	0.902 (2)
C12	0.61913 (9)	0.8524 (3)	0.42467 (9)	0.0477 (4)	0.902 (2)
C13	0.56757 (15)	0.8395 (5)	0.34734 (11)	0.0692 (7)	0.902 (2)
H13A	0.5325	0.7151	0.3367	0.104*	0.902 (2)
H13B	0.5959	0.8129	0.3236	0.104*	0.902 (2)
H13C	0.5402	0.9821	0.3306	0.104*	0.902 (2)
O2A	0.6546 (18)	1.057 (4)	0.4397 (12)	0.0586 (6)	0.098 (2)
C9A	0.6013 (8)	0.735 (3)	0.4376 (7)	0.0427 (4)	0.098 (2)
C10A	0.5807 (13)	0.803 (3)	0.3684 (9)	0.0531 (5)	0.098 (2)
H10B	0.5522	0.7164	0.3268	0.064*	0.098 (2)
C11A	0.6069 (10)	1.005 (3)	0.3706 (8)	0.0595 (5)	0.098 (2)
H11B	0.5950	1.0994	0.3313	0.071*	0.098 (2)
C12A	0.6552 (8)	0.873 (3)	0.4795 (7)	0.0477 (4)	0.098 (2)
C13A	0.7071 (16)	0.887 (5)	0.5558 (9)	0.0692 (7)	0.098 (2)
H13D	0.6946	0.7703	0.5798	0.104*	0.098 (2)
H13E	0.7035	1.0362	0.5730	0.104*	0.098 (2)
H13F	0.7578	0.8623	0.5656	0.104*	0.098 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0482 (6)	0.0443 (6)	0.0459 (6)	−0.0052 (5)	0.0218 (5)	0.0039 (5)

N1	0.0484 (7)	0.0478 (8)	0.0391 (6)	−0.0095 (6)	0.0100 (6)	0.0062 (5)
N2	0.0426 (6)	0.0444 (7)	0.0432 (7)	−0.0068 (6)	0.0107 (5)	0.0049 (5)
N3	0.0432 (7)	0.0462 (7)	0.0517 (7)	−0.0071 (6)	0.0142 (6)	0.0022 (6)
C1	0.0402 (7)	0.0474 (8)	0.0375 (7)	−0.0003 (6)	0.0143 (6)	0.0014 (6)
C2	0.0646 (11)	0.0627 (11)	0.0479 (9)	−0.0138 (9)	0.0096 (8)	0.0120 (8)
C3	0.0753 (13)	0.0787 (14)	0.0491 (10)	−0.0088 (11)	0.0130 (9)	0.0186 (9)
C4	0.0603 (10)	0.0847 (14)	0.0358 (8)	−0.0021 (10)	0.0133 (7)	0.0004 (8)
C5	0.0600 (10)	0.0728 (12)	0.0442 (9)	−0.0170 (9)	0.0178 (8)	−0.0097 (8)
C6	0.0565 (9)	0.0570 (10)	0.0412 (8)	−0.0096 (8)	0.0184 (7)	0.0001 (7)
C7	0.0405 (7)	0.0390 (7)	0.0428 (7)	−0.0014 (6)	0.0175 (6)	0.0042 (6)
C8	0.0381 (7)	0.0442 (8)	0.0529 (9)	−0.0039 (6)	0.0199 (6)	−0.0035 (7)
O2	0.0619 (15)	0.0533 (10)	0.0601 (9)	−0.0143 (10)	0.0305 (9)	0.0024 (7)
C9	0.0386 (8)	0.0426 (9)	0.0437 (9)	−0.0037 (7)	0.0185 (7)	−0.0017 (7)
C10	0.0490 (11)	0.0551 (13)	0.0472 (10)	−0.0105 (9)	0.0185 (9)	−0.0030 (8)
C11	0.0592 (11)	0.0577 (11)	0.0534 (11)	−0.0206 (9)	0.0224 (9)	−0.0110 (9)
C12	0.0473 (9)	0.0465 (10)	0.0488 (9)	−0.0075 (8)	0.0240 (8)	−0.0018 (7)
C13	0.0665 (15)	0.0825 (17)	0.0459 (12)	−0.0067 (13)	0.0193 (11)	0.0064 (11)
O2A	0.0619 (15)	0.0533 (10)	0.0601 (9)	−0.0143 (10)	0.0305 (9)	0.0024 (7)
C9A	0.0386 (8)	0.0426 (9)	0.0437 (9)	−0.0037 (7)	0.0185 (7)	−0.0017 (7)
C10A	0.0490 (11)	0.0551 (13)	0.0472 (10)	−0.0105 (9)	0.0185 (9)	−0.0030 (8)
C11A	0.0592 (11)	0.0577 (11)	0.0534 (11)	−0.0206 (9)	0.0224 (9)	−0.0110 (9)
C12A	0.0473 (9)	0.0465 (10)	0.0488 (9)	−0.0075 (8)	0.0240 (8)	−0.0018 (7)
C13A	0.0665 (15)	0.0825 (17)	0.0459 (12)	−0.0067 (13)	0.0193 (11)	0.0064 (11)

Geometric parameters (Å, º)

O1—C7	1.3592 (18)	O2—C12	1.370 (3)
O1—C8	1.3938 (18)	C9—C12	1.355 (2)
N1—C7	1.3388 (19)	C9—C10	1.433 (2)
N1—C1	1.4040 (19)	C10—C11	1.318 (3)
N1—H1N	0.919 (19)	C10—H10A	0.9500
N2—C7	1.2947 (19)	C11—H11A	0.9500
N2—N3	1.4049 (18)	C12—C13	1.484 (3)
N3—C8	1.270 (2)	C13—H13A	0.9800
C1—C2	1.379 (2)	C13—H13B	0.9800
C1—C6	1.385 (2)	C13—H13C	0.9800
C2—C3	1.384 (2)	O2A—C11A	1.363 (19)
C2—H2A	0.9500	O2A—C12A	1.391 (16)
C3—C4	1.366 (3)	C9A—C12A	1.317 (14)
C3—H3A	0.9500	C9A—C10A	1.415 (16)
C4—C5	1.366 (3)	C10A—C11A	1.304 (17)
C4—H4A	0.9500	C10A—H10B	0.9500
C5—C6	1.382 (2)	C11A—H11B	0.9500
C5—H5A	0.9500	C12A—C13A	1.468 (12)
C6—H6A	0.9500	C13A—H13D	0.9800
C8—C9	1.446 (2)	C13A—H13E	0.9800
C8—C9A	1.649 (15)	C13A—H13F	0.9800
O2—C11	1.369 (3)		

C7—O1—C8	101.65 (11)	C10—C9—C8	124.36 (16)
C7—N1—C1	130.48 (14)	C11—C10—C9	106.53 (19)
C7—N1—H1N	114.2 (11)	C11—C10—H10A	126.7
C1—N1—H1N	114.9 (11)	C9—C10—H10A	126.7
C7—N2—N3	106.47 (12)	C10—C11—O2	110.83 (18)
C8—N3—N2	106.56 (12)	C10—C11—H11A	124.6
C2—C1—C6	119.18 (15)	O2—C11—H11A	124.6
C2—C1—N1	125.04 (15)	C9—C12—O2	108.78 (17)
C6—C1—N1	115.78 (14)	C9—C12—C13	135.13 (18)
C1—C2—C3	119.50 (18)	O2—C12—C13	116.09 (19)
C1—C2—H2A	120.3	C12—C13—H13A	109.5
C3—C2—H2A	120.3	C12—C13—H13B	109.5
C4—C3—C2	121.35 (19)	H13A—C13—H13B	109.5
C4—C3—H3A	119.3	C12—C13—H13C	109.5
C2—C3—H3A	119.3	H13A—C13—H13C	109.5
C3—C4—C5	119.16 (16)	H13B—C13—H13C	109.5
C3—C4—H4A	120.4	C11A—O2A—C12A	107.1 (15)
C5—C4—H4A	120.4	C12A—C9A—C10A	105.2 (13)
C4—C5—C6	120.62 (17)	C12A—C9A—C8	111.3 (11)
C4—C5—H5A	119.7	C10A—C9A—C8	142.6 (12)
C6—C5—H5A	119.7	C11A—C10A—C9A	109.1 (14)
C5—C6—C1	120.18 (17)	C11A—C10A—H10B	125.4
C5—C6—H6A	119.9	C9A—C10A—H10B	125.4
C1—C6—H6A	119.9	C10A—C11A—O2A	107.7 (14)
N2—C7—N1	125.19 (14)	C10A—C11A—H11B	126.2
N2—C7—O1	112.65 (13)	O2A—C11A—H11B	126.2
N1—C7—O1	122.14 (13)	C9A—C12A—O2A	108.2 (13)
N3—C8—O1	112.66 (14)	C9A—C12A—C13A	135.1 (16)
N3—C8—C9	126.35 (15)	O2A—C12A—C13A	116.3 (16)
O1—C8—C9	120.97 (14)	C12A—C13A—H13D	109.5
N3—C8—C9A	156.6 (5)	C12A—C13A—H13E	109.5
O1—C8—C9A	90.7 (5)	H13D—C13A—H13E	109.5
C11—O2—C12	107.00 (19)	C12A—C13A—H13F	109.5
C12—C9—C10	106.85 (16)	H13D—C13A—H13F	109.5
C12—C9—C8	128.78 (16)	H13E—C13A—H13F	109.5
C7—N2—N3—C8	0.33 (17)	O1—C8—C9—C10	178.34 (18)
C7—N1—C1—C2	0.8 (3)	C12—C9—C10—C11	−0.2 (2)
C7—N1—C1—C6	−178.43 (16)	C8—C9—C10—C11	179.94 (18)
C6—C1—C2—C3	−0.5 (3)	C9—C10—C11—O2	0.1 (3)
N1—C1—C2—C3	−179.69 (18)	C12—O2—C11—C10	0.1 (3)
C1—C2—C3—C4	0.4 (3)	C10—C9—C12—O2	0.3 (2)
C2—C3—C4—C5	0.2 (3)	C8—C9—C12—O2	−179.9 (2)
C3—C4—C5—C6	−0.8 (3)	C10—C9—C12—C13	−179.8 (3)
C4—C5—C6—C1	0.7 (3)	C8—C9—C12—C13	0.0 (4)
C2—C1—C6—C5	0.0 (3)	C11—O2—C12—C9	−0.2 (3)
N1—C1—C6—C5	179.21 (16)	C11—O2—C12—C13	179.9 (2)

N3—N2—C7—N1	177.98 (15)	N3—C8—C9A—C12A	4 (2)
N3—N2—C7—O1	−0.07 (17)	O1—C8—C9A—C12A	179.1 (12)
C1—N1—C7—N2	170.37 (16)	N3—C8—C9A—C10A	171 (2)
C1—N1—C7—O1	−11.8 (3)	O1—C8—C9A—C10A	−14 (3)
C8—O1—C7—N2	−0.19 (16)	C12A—C9A—C10A—C11A	−16 (3)
C8—O1—C7—N1	−178.30 (14)	C8—C9A—C10A—C11A	176.6 (18)
N2—N3—C8—O1	−0.47 (17)	C9A—C10A—C11A—O2A	10 (3)
N2—N3—C8—C9	177.97 (15)	C12A—O2A—C11A—C10A	0 (4)
N2—N3—C8—C9A	173.9 (14)	C10A—C9A—C12A—O2A	16 (3)
C7—O1—C8—N3	0.41 (17)	C8—C9A—C12A—O2A	−173 (2)
C7—O1—C8—C9	−178.11 (14)	C10A—C9A—C12A—C13A	−172 (3)
C7—O1—C8—C9A	−177.3 (6)	C8—C9A—C12A—C13A	−1 (3)
N3—C8—C9—C12	−179.81 (17)	C11A—O2A—C12A—C9A	−10 (3)
O1—C8—C9—C12	−1.5 (3)	C11A—O2A—C12A—C13A	176 (3)
N3—C8—C9—C10	0.0 (3)		

Hydrogen-bond geometry (Å, º)

Cg3, Cg2 are the centroid of benzene (C1–C6) and furan (O2/C9–C12) rings, respectively.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1N⋯N2[i]	0.92 (2)	1.97 (2)	2.885 (2)	171 (2)
C2—H2A⋯O1	0.95	2.31	2.930 (2)	122
C13—H13A⋯O1	0.98	2.46	3.151 (3)	127
C13A—H13D⋯N3	0.98	2.65	3.41 (3)	134
C5—H5A⋯Cg3[ii]	0.95	2.89	3.655 (4)	138
C13A—H13F⋯Cg2[iii]	0.98	2.80	3.612 (8)	141

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