

## Crystal structure of 5-(furan-2-yl)-*N*-phenyl-1,3,4-oxadiazol-2-amine

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The title compound, C<sub>12</sub>H<sub>9</sub>N<sub>3</sub>O<sub>2</sub>, was obtained as a cyclized oxadiazole derivative from substituted thiosemicarbazide in the presence of manganese(II) acetate. The furan ring is disordered over two orientations, with occupancies of 0.76 (2) and 0.24 (2). The dihedral angles between the central oxadiazole ring and the pendant phenyl ring and furan ring (major disorder component) are 3.34 (18) and 5.7 (6)°, 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*<sub>2</sub><sup>2</sup>[8] loops. The dimers are linked by C—H···π and π—π interactions [range of centroid—centroid distances = 3.291 (2)–3.460 (8) Å], generating a three-dimensional network.

**Keywords:** crystal structure; cyclized oxadiazole derivative; hydrogen bonding; C—H···π interactions; π—π interactions.

**CCDC reference:** 1431289

### 1. Related literature

For heterocyclic ligands that form metal complexes, see: Tarafder *et al.* (2001); Ali & Ali (2007); Singh *et al.* (2007); Zhao *et al.* (2007); Zhang *et al.* (2007); Amin *et al.* (2004). For applications in medicine and agriculture, see: Pachhamia & Parikh (1988); Xu *et al.* (2002). For related structures, see: Foks *et al.* (2002); Dani *et al.* (2013).

### 2. Experimental

#### 2.1. Crystal data

C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	<i>V</i> = 1060.0 (3) Å <sup>3</sup>
<i>M<sub>r</sub></i> = 227.22	<i>Z</i> = 4
Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>	Mo <i>K</i> α radiation
<i>a</i> = 13.195 (3) Å	<i>μ</i> = 0.10 mm <sup>-1</sup>
<i>b</i> = 5.6162 (8) Å	<i>T</i> = 293 K
<i>c</i> = 14.958 (3) Å	0.4 × 0.3 × 0.15 mm
<i>β</i> = 107.00 (2)°	

#### 2.2. Data collection

Agilent Xcalibur Eos diffractometer	4305 measured reflections
Absorption correction: multi-scan ( <i>CrysAlis PRO</i> ; Agilent, 2011)	2405 independent reflections
<i>T</i> <sub>min</sub> = 0.941, <i>T</i> <sub>max</sub> = 1.000	1057 reflections with <i>I</i> > 2σ( <i>I</i> )
	<i>R</i> <sub>int</sub> = 0.039

#### 2.3. Refinement

<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.064	H atoms treated by a mixture of independent and constrained refinement
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.142	<i>Δρ</i> <sub>max</sub> = 0.19 e Å <sup>-3</sup>
<i>S</i> = 1.01	<i>Δρ</i> <sub>min</sub> = -0.21 e Å <sup>-3</sup>
2405 reflections	
174 parameters	
40 restraints	

**Table 1**

Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*4 are the centroids of the O1A/C1/C2/C3/C4 and C7–C12 five- and six-membered rings, respectively.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N3—H3N3···N2 <sup>i</sup>	1.02 (3)	1.87 (3)	2.892 (3)	178 (2)
C12—H12A···O2	0.93	2.27	2.892 (4)	123
C9—H9A···Cg1 <sup>ii</sup>	0.93	3.00	3.653 (4)	129
C2—H2A···Cg4 <sup>iii</sup>	0.93	2.93	3.664 (5)	137

Symmetry codes: (i)  $-x + 1, -y + 2, -z + 1$ ; (ii)  $x - \frac{1}{2}, -y - \frac{1}{2}, z - \frac{1}{2}$ ; (iii)  $x - \frac{3}{2}, -y + \frac{1}{2}, z - \frac{3}{2}$ .

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

### Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7522).

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## References

- Agilent (2011). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
- Ali, S. & Ali, R. (2007). *Tetrahedron Lett.* **48**, 1549–1551.
- Amin, O. H., Al-Hayaly, L. J., Al-Jibori, S. A. & Al-Allaf, T. A. K. (2004). *Polyhedron*, **23**, 2013–2020.
- Dani, R. K., Bharty, M. K., Kushawaha, S. K., Paswan, S., Prakash, O., Singh, N. K. & Singh, N. K. (2013). *J. Mol. Struct.* **1054–1055**, 251–261.
- Foks, H., Mieczkowska, J., Janowiec, M., Zwolska, Z. & Andrzejczyk, Z. (2002). *Chem. Heterocycl. Compd.* **38**, 810–816.
- Pachhamia, V. L. & Parikh, A. R. (1988). *J. Indian Chem. Soc.* **65**, 357–361.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Singh, N. K., Butcher, R. J., Tripathi, P., Srivastava, A. K. & Bharty, M. K. (2007). *Acta Cryst.* **E63**, o782–o784.
- Tarafder, Md. T. H., Saravanan, N., Crouse, K. A. & Ali, A. M. b. (2001). *Transition Met. Chem.* **26**, 613–618.
- Xu, L. Z., Jiao, K., Zhang, S. S. & Kuang, S. P. (2002). *Bull. Korean. Chem. Soc.* **23**, 1699–1701.
- Zhang, Z.-H., Tian, Y.-L. & Guo, Y.-M. (2007). *Inorg. Chim. Acta*, **360**, 2783–2788.
- Zhao, X.-X., Ma, J.-P., Dong, Y. B., Huang, R.-Q. & Lai, T. (2007). *Cryst. Growth Des.* **7**, 1058–1068.

## supporting information

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Crystal structure of 5-(furan-2-yl)-*N*-phenyl-1,3,4-oxadiazol-2-amine

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## S1. Comment

1,3,4-Oxadiazole-2-thiones, an important class of heterocyclic ligands in the field of coordination chemistry (Tarafder *et al.*, 2001; Ali & Ali, 2007; Singh *et al.*, 2007; Zhao *et al.*, 2007; Zhang *et al.*, 2007; Amin *et al.*, 2004) have wide applications both in medicine and agriculture (Pachhamia & Parikh, 1988; Xu *et al.*, 2002). The cyclization of 3-acyl-dithiocarbamate esters, *N*-aroyldithiocarbamates and their salts to the corresponding 1,3,4-oxadiazole in the presence of base is reported in the literature (Foks *et al.*, 2002). Further, 5-benzyl-*N*-phenyl-1,3,4-thiadiazole-2-amine and 2-(5-phenyl-1,3,4-thiadiazol-2-yl)pyridine have also been reported in the presence of manganese(II) nitrate *via* loss of H<sub>2</sub>O (Dani *et al.*, 2013). It is known that in the presence of strong acid, *N*-acylhydrazine carbodithioate is converted into thiadiazole but in presence of weak acid or base they are cyclized into oxadiazole. In the present case, manganese(II) acetate behaves like a weak acid and thus converts thiosemicarbazide into oxadiazole *via* loss of H<sub>2</sub>S.

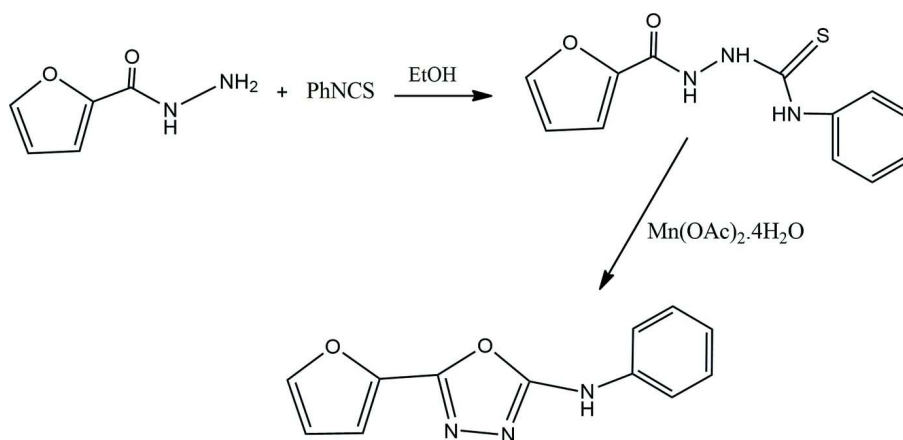
In the title compound (Fig. 2), the mean plane of the central oxadiazole ring (O2/C5/N1/N2/C6) forms dihedral angles of 5.65 and 3.34° with the furan (O1/C1–C4) and phenyl rings (C7–C12), respectively. Both the furan and phenyl rings are twisted by an angle of 7.51°. The C–N bond lengths, N1–C5 1.290 (4) and N2–C6 1.302 (4) Å, are similar to standard C=N 1.28 Å. The distances found within the oxadiazole ring are intermediate between single and double bond, suggesting considerable delocalization in the ring. In the crystal, pairs of intermolecular N—H⋯N hydrogen bonds between the oxadiazole ring and the amine group forming dimers with an R<sub>2</sub><sup>2</sup>[8] ring motif (Fig. 3, Table 1) and an intramolecular C—H⋯O interaction is also found. Molecules are further linked by weak C—H⋯N and two C—H⋯π interactions, involving (C7–C12) and (O1/C1–C4) rings. In addition, weak π⋯π intermolecular stacking interactions [Cg1⋯Cg2 (x, 1+y, z) = 3.460 (8)Å; Cg2⋯Cg2 (1-x, 1-y, 1-z) = 3.291 (2)Å; Cg2⋯Cg3 (x, -1+y, z) = 3.431 (4)Å; Cg1: O1/C1–C4; Cg2: O2/C5/N1/N2/C6; Cg3: O1A/C1A–C4A] are present and influences the crystal packing. The furan ring is disordered over two positions, with occupancies of 0.76 (2) and 0.24 (2).

## S2. Experimental

Referring to Fig. 1, a mixture of furan-2-carboxylic acid hydrazide (1.260 g, 10 mmol) and phenyl isothiocyanate (1.2 ml, 10 mmol) in absolute ethanol (20 mL) was refluxed for 4 h. The solid *N*-(furan-2-carbonyl)-4-phenylthiosemicarbazide obtained upon cooling was filtered off and washed with water and ether (50:50 v/v). A mixture of methanolic solution of *N*-(furan-2-carbonyl)-4-phenylthiosemicarbazide (0.261 g, 1.00 mmol) and Mn(OAc)<sub>2</sub>·4H<sub>2</sub>O (0.246 g, 1 mmol) was stirred for 4 h. A clear yellow solution obtained was filtered off and kept for crystallization. Colourless needles were obtained after 10 days. Yield: 60%; m.p.: 476–478 K. Anal. Calc. for C<sub>12</sub>H<sub>9</sub>N<sub>3</sub>O<sub>2</sub>(%): C 63.43, H 3.99, N 18.49. Found: C 63.68, H 4.05, N 18.61. <sup>1</sup>H NMR (DMSO-d<sub>6</sub>): δ [ppm] = 11.60 (s, 1H, NH), 8.80–7.31 (m, 3H, furan), 7.80–6.76 (m, 5H, Phenyl). <sup>13</sup>C NMR (DMSO-d<sub>6</sub>): δ [ppm] = 161.3 (C6), 162.0 (C5), 153.7 (C4), 146.9 (C1), 144.8 (C3), 140.7 (C2) (furan C); 120.6–145.2 (phenyl C) (Fig. 2). IR (selected, KBr): 3210 [ν(N–H)], 1605 [ν(C=N)], 1076 [ν(N–N)] cm<sup>-1</sup>.

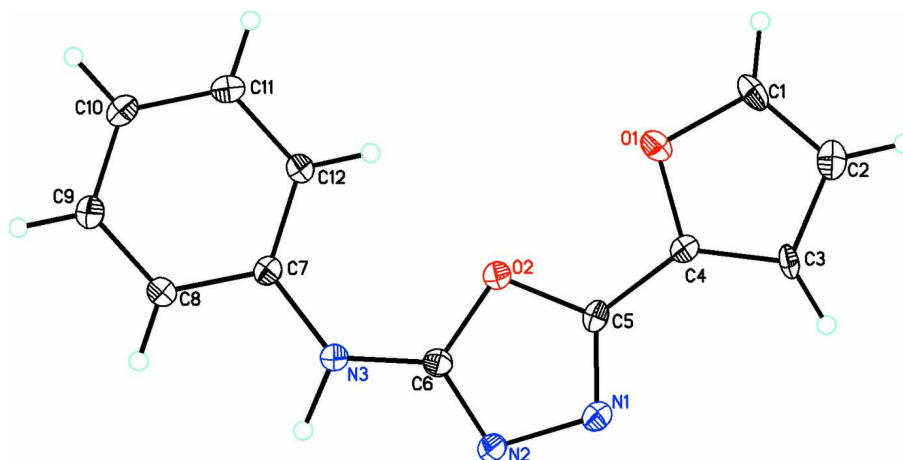
### S3. Refinement

The H atom bonded to N3 was located in a difference Fourier map and refined freely; N3–H3N3 = 1.02 (3) Å. Other H atoms were positioned geometrically and allowed to ride on their parent atoms, with C–H = 0.93 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The ISOR restraint and EADP constraint commands in the *SHELXL2014* software were used for the disordered atoms.



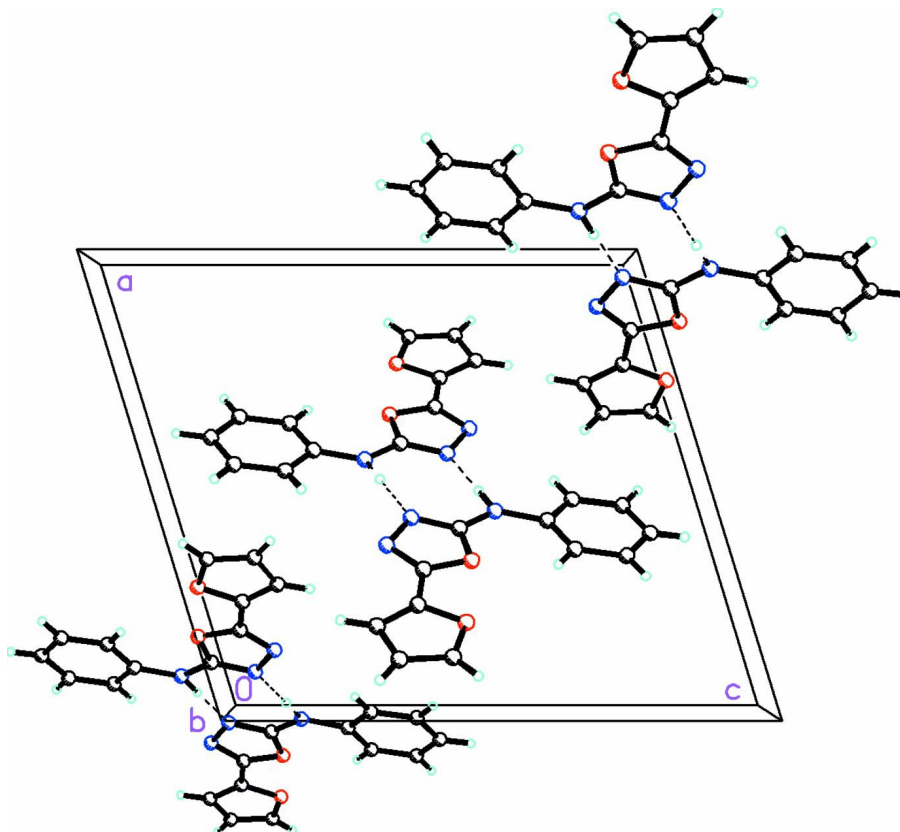
**Figure 1**

Scheme showing the synthesis of the title compound.



**Figure 2**

The molecular structure of (I) showing 50% probability displacement ellipsoids.



**Figure 3**

The molecular packing of the title compound, viewed along the *b*-axis. Dashed lines indicate weak N—H...N intermolecular hydrogen bonding between the oxadiazole ring and the amine group, forming dimers with an  $R^2_2[8]$  ring motif.

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

#### Crystal data

$C_{12}H_9N_3O_2$

$M_r = 227.22$

Monoclinic,  $P2_1/n$

$a = 13.195$  (3) Å

$b = 5.6162$  (8) Å

$c = 14.958$  (3) Å

$\beta = 107.00$  (2)°

$V = 1060.0$  (3) Å<sup>3</sup>

$Z = 4$

$F(000) = 472$

$D_x = 1.424$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 594 reflections

$\theta = 3.1$ – $29.0$ °

$\mu = 0.10$  mm<sup>-1</sup>

$T = 293$  K

Needle, colourless

$0.4 \times 0.3 \times 0.15$  mm

#### Data collection

Agilent Xcalibur Eos  
diffractometer

Radiation source: Enhance (Mo) X-ray Source  
Graphite monochromator

Detector resolution: 16.0938 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan  
(*CrysAlis PRO*; Agilent, 2011)

$T_{\min} = 0.941$ ,  $T_{\max} = 1.000$

4305 measured reflections

2405 independent reflections

1057 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 29.1^\circ$ ,  $\theta_{\min} = 3.2^\circ$   
 $h = -18 \rightarrow 13$

$k = -7 \rightarrow 7$   
 $l = -19 \rightarrow 17$

### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.064$   
 $wR(F^2) = 0.142$   
 $S = 1.01$   
 2405 reflections  
 174 parameters  
 40 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: mixed  
 H atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0308P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.19 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$

### 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 on  $F^2$  for ALL reflections except those flagged by the user for potential systematic errors. Weighted  $R$ -factors  $wR$  and all goodnesses 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 observed criterion of  $F^2 > \sigma(F^2)$  is used only for calculating  $-R$ -factor-obs *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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O2	0.65450 (17)	0.5460 (3)	0.46696 (13)	0.0425 (6)	
N1	0.6233 (2)	0.5577 (4)	0.60530 (17)	0.0463 (7)	
N2	0.5682 (2)	0.7470 (4)	0.54975 (17)	0.0445 (7)	
N3	0.5544 (2)	0.8799 (4)	0.39788 (17)	0.0449 (7)	
H3N3	0.512 (2)	1.014 (5)	0.4150 (19)	0.067 (11)*	
O1	0.7733 (7)	0.1580 (16)	0.5086 (4)	0.0560 (14)	0.76 (2)
C1	0.8374 (6)	-0.0405 (14)	0.5478 (9)	0.057 (2)	0.76 (2)
H1A	0.8716	-0.1392	0.5158	0.068*	0.76 (2)
C2	0.8412 (7)	-0.0643 (15)	0.6370 (8)	0.062 (2)	0.76 (2)
H2A	0.8780	-0.1815	0.6776	0.074*	0.76 (2)
C3	0.7797 (8)	0.1194 (18)	0.6598 (6)	0.0470 (17)	0.76 (2)
H3A	0.7692	0.1477	0.7177	0.056*	0.76 (2)
C4	0.740 (2)	0.244 (4)	0.5812 (9)	0.0395 (13)	0.76 (2)
O1A	0.790 (3)	0.093 (5)	0.5177 (17)	0.0560 (14)	0.24 (2)
C1A	0.844 (3)	-0.073 (5)	0.587 (2)	0.057 (2)	0.24 (2)
H1AA	0.8868	-0.1956	0.5766	0.068*	0.24 (2)
C2A	0.826 (3)	-0.029 (5)	0.6672 (18)	0.062 (2)	0.24 (2)
H2AA	0.8545	-0.1113	0.7226	0.074*	0.24 (2)
C3A	0.755 (3)	0.163 (6)	0.655 (2)	0.0470 (17)	0.24 (2)
H3AA	0.7244	0.2242	0.6989	0.056*	0.24 (2)
C4A	0.741 (8)	0.238 (13)	0.568 (3)	0.0395 (13)	0.24 (2)
C5	0.6717 (3)	0.4467 (5)	0.5543 (2)	0.0411 (8)	

C6	0.5901 (3)	0.7321 (5)	0.4705 (2)	0.0409 (8)
C7	0.5742 (3)	0.8830 (5)	0.3105 (2)	0.0408 (8)
C8	0.5304 (3)	1.0704 (5)	0.2521 (2)	0.0515 (9)
H8A	0.4916	1.1860	0.2722	0.062*
C9	0.5436 (3)	1.0878 (6)	0.1647 (2)	0.0627 (11)
H9A	0.5129	1.2139	0.1259	0.075*
C10	0.6013 (3)	0.9215 (6)	0.1342 (2)	0.0607 (11)
H10A	0.6097	0.9332	0.0748	0.073*
C11	0.6470 (3)	0.7360 (6)	0.1925 (2)	0.0593 (10)
H11A	0.6876	0.6238	0.1727	0.071*
C12	0.6330 (3)	0.7158 (5)	0.2798 (2)	0.0518 (9)
H12A	0.6633	0.5889	0.3183	0.062*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O2	0.0432 (14)	0.0445 (12)	0.0412 (12)	0.0048 (11)	0.0147 (11)	0.0035 (9)
N1	0.0496 (18)	0.0517 (15)	0.0372 (15)	-0.0012 (15)	0.0123 (14)	-0.0020 (12)
N2	0.0463 (18)	0.0501 (16)	0.0384 (15)	0.0039 (14)	0.0146 (14)	0.0015 (12)
N3	0.0511 (19)	0.0456 (16)	0.0418 (16)	0.0102 (14)	0.0192 (15)	0.0040 (12)
O1	0.061 (3)	0.044 (4)	0.065 (2)	0.017 (3)	0.022 (2)	0.006 (2)
C1	0.049 (3)	0.036 (3)	0.081 (6)	0.014 (2)	0.014 (4)	0.012 (4)
C2	0.060 (4)	0.064 (3)	0.055 (5)	0.001 (3)	0.007 (4)	0.014 (4)
C3	0.043 (5)	0.048 (4)	0.042 (2)	0.017 (3)	-0.001 (3)	0.017 (2)
C4	0.042 (2)	0.043 (2)	0.035 (4)	-0.0025 (17)	0.013 (5)	-0.002 (4)
O1A	0.061 (3)	0.044 (4)	0.065 (2)	0.017 (3)	0.022 (2)	0.006 (2)
C1A	0.049 (3)	0.036 (3)	0.081 (6)	0.014 (2)	0.014 (4)	0.012 (4)
C2A	0.060 (4)	0.064 (3)	0.055 (5)	0.001 (3)	0.007 (4)	0.014 (4)
C3A	0.043 (5)	0.048 (4)	0.042 (2)	0.017 (3)	-0.001 (3)	0.017 (2)
C4A	0.042 (2)	0.043 (2)	0.035 (4)	-0.0025 (17)	0.013 (5)	-0.002 (4)
C5	0.042 (2)	0.0453 (18)	0.0321 (17)	-0.0056 (17)	0.0056 (16)	0.0040 (14)
C6	0.039 (2)	0.0412 (18)	0.0430 (19)	-0.0004 (16)	0.0122 (16)	-0.0018 (15)
C7	0.041 (2)	0.0437 (18)	0.0377 (18)	-0.0019 (17)	0.0112 (16)	0.0004 (14)
C8	0.062 (2)	0.0446 (19)	0.052 (2)	0.0121 (18)	0.023 (2)	0.0051 (16)
C9	0.079 (3)	0.062 (2)	0.052 (2)	0.020 (2)	0.026 (2)	0.0165 (17)
C10	0.073 (3)	0.070 (2)	0.047 (2)	0.010 (2)	0.030 (2)	0.0091 (18)
C11	0.070 (3)	0.061 (2)	0.056 (2)	0.013 (2)	0.033 (2)	-0.0006 (18)
C12	0.058 (2)	0.0509 (19)	0.051 (2)	0.0180 (19)	0.0230 (19)	0.0114 (16)

*Geometric parameters (Å, °)*

O2—C6	1.358 (3)	C1A—C2A	1.321 (16)
O2—C5	1.376 (3)	C1A—H1AA	0.9300
N1—C5	1.290 (4)	C2A—C3A	1.397 (16)
N1—N2	1.413 (3)	C2A—H2AA	0.9300
N2—C6	1.302 (4)	C3A—C4A	1.335 (16)
N3—C6	1.339 (3)	C3A—H3AA	0.9300
N3—C7	1.406 (4)	C4A—C5	1.46 (2)

N3—H3N3	1.02 (3)	C7—C12	1.379 (4)
O1—C4	1.375 (6)	C7—C8	1.382 (4)
O1—C1	1.418 (6)	C8—C9	1.371 (4)
C1—C2	1.328 (7)	C8—H8A	0.9300
C1—H1A	0.9300	C9—C10	1.365 (4)
C2—C3	1.414 (7)	C9—H9A	0.9300
C2—H2A	0.9300	C10—C11	1.379 (4)
C3—C4	1.337 (6)	C10—H10A	0.9300
C3—H3A	0.9300	C11—C12	1.376 (4)
C4—C5	1.433 (8)	C11—H11A	0.9300
O1A—C4A	1.387 (16)	C12—H12A	0.9300
O1A—C1A	1.418 (16)		
C6—O2—C5	101.9 (2)	C3A—C4A—O1A	112.9 (16)
C5—N1—N2	105.9 (2)	C3A—C4A—C5	107 (2)
C6—N2—N1	105.9 (3)	O1A—C4A—C5	140 (3)
C6—N3—C7	130.2 (3)	N1—C5—O2	113.1 (3)
C6—N3—H3N3	110.1 (16)	N1—C5—C4	126.5 (5)
C7—N3—H3N3	119.5 (16)	O2—C5—C4	120.3 (5)
C4—O1—C1	103.9 (5)	N1—C5—C4A	134.6 (14)
C2—C1—O1	109.7 (5)	O2—C5—C4A	112.2 (13)
C2—C1—H1A	125.1	N2—C6—N3	125.4 (3)
O1—C1—H1A	125.1	N2—C6—O2	113.2 (3)
C1—C2—C3	108.3 (5)	N3—C6—O2	121.4 (3)
C1—C2—H2A	125.9	C12—C7—C8	118.7 (3)
C3—C2—H2A	125.9	C12—C7—N3	125.2 (3)
C4—C3—C2	106.1 (5)	C8—C7—N3	116.1 (3)
C4—C3—H3A	127.0	C9—C8—C7	120.7 (3)
C2—C3—H3A	127.0	C9—C8—H8A	119.6
C3—C4—O1	112.1 (6)	C7—C8—H8A	119.6
C3—C4—C5	135.8 (8)	C10—C9—C8	120.6 (3)
O1—C4—C5	112.1 (8)	C10—C9—H9A	119.7
C4A—O1A—C1A	102.0 (14)	C8—C9—H9A	119.7
C2A—C1A—O1A	110.6 (15)	C9—C10—C11	119.2 (3)
C2A—C1A—H1AA	124.7	C9—C10—H10A	120.4
O1A—C1A—H1AA	124.7	C11—C10—H10A	120.4
C1A—C2A—C3A	108.7 (16)	C12—C11—C10	120.5 (3)
C1A—C2A—H2AA	125.6	C12—C11—H11A	119.8
C3A—C2A—H2AA	125.6	C10—C11—H11A	119.8
C4A—C3A—C2A	105.5 (16)	C11—C12—C7	120.3 (3)
C4A—C3A—H3AA	127.3	C11—C12—H12A	119.9
C2A—C3A—H3AA	127.3	C7—C12—H12A	119.9
C5—N1—N2—C6	-0.7 (3)	C3—C4—C5—O2	173 (3)
C4—O1—C1—C2	-0.7 (18)	O1—C4—C5—O2	-6 (3)
O1—C1—C2—C3	-0.2 (11)	C3A—C4A—C5—N1	-2 (12)
C1—C2—C3—C4	1.1 (19)	O1A—C4A—C5—N1	173 (9)
C2—C3—C4—O1	-2 (3)	C3A—C4A—C5—O2	178 (5)



C2—C3—C4—C5	179 (3)	O1A—C4A—C5—O2	-7 (15)
C1—O1—C4—C3	1 (3)	N1—N2—C6—N3	-179.4 (3)
C1—O1—C4—C5	-179.2 (18)	N1—N2—C6—O2	0.9 (3)
C4A—O1A—C1A—C2A	1 (7)	C7—N3—C6—N2	178.8 (3)
O1A—C1A—C2A—C3A	2 (5)	C7—N3—C6—O2	-1.5 (5)
C1A—C2A—C3A—C4A	-5 (7)	C5—O2—C6—N2	-0.7 (3)
C2A—C3A—C4A—O1A	6 (10)	C5—O2—C6—N3	179.6 (3)
C2A—C3A—C4A—C5	-177 (5)	C6—N3—C7—C12	4.1 (5)
C1A—O1A—C4A—C3A	-5 (9)	C6—N3—C7—C8	-175.8 (3)
C1A—O1A—C4A—C5	-180 (12)	C12—C7—C8—C9	1.1 (5)
N2—N1—C5—O2	0.2 (3)	N3—C7—C8—C9	-178.9 (3)
N2—N1—C5—C4	178.7 (18)	C7—C8—C9—C10	-0.8 (6)
N2—N1—C5—C4A	-180 (7)	C8—C9—C10—C11	-0.4 (6)
C6—O2—C5—N1	0.3 (3)	C9—C10—C11—C12	1.3 (6)
C6—O2—C5—C4	-178.3 (17)	C10—C11—C12—C7	-0.9 (6)
C6—O2—C5—C4A	-180 (5)	C8—C7—C12—C11	-0.3 (5)
C3—C4—C5—N1	-5 (5)	N3—C7—C12—C11	179.8 (3)
O1—C4—C5—N1	175.9 (13)		

*Hydrogen-bond geometry (Å, °)*

Cg1 and Cg4 are the centroids of the O1A/C1/C2/C3/C4 and C7—C12 five- and six-membered rings, respectively.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N3—H3N3...N2 <sup>i</sup>	1.02 (3)	1.87 (3)	2.892 (3)	178 (2)
C12—H12A...O2	0.93	2.27	2.892 (4)	123
C9—H9A...Cg1 <sup>ii</sup>	0.93	3.00	3.653 (4)	129
C2—H2A...Cg4 <sup>iii</sup>	0.93	2.93	3.664 (5)	137

Symmetry codes: (i)  $-x+1, -y+2, -z+1$ ; (ii)  $x-1/2, -y-1/2, z-1/2$ ; (iii)  $x-3/2, -y+1/2, z-3/2$ .