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# (2*E*)-2-(4-Hydroxy-3-methoxybenzylidene)hydrazinecarboxamide

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Key indicators: single-crystal X-ray study; T = 296 K; mean  $\sigma$ (C–C) = 0.009 Å; R factor = 0.056; wR factor = 0.113; data-to-parameter ratio = 7.0.

In the title compound,  $C_9H_{11}N_3O_3$ , two molecules are present in the asymmetric unit in which the 4-hydroxy-3-methoxybenzaldehyde and hydrazinecarboxamide units are almost planar [with r.m.s. deviations 0.0212 and 0.0066 Å, respectively, in one molecule and 0.0346 and 0.0095 Å, respectively, in the other] and are oriented at dihedral angles of 9.7 (3) and 16.6 (3)°. In both molecules, two S(5) ring motifs are present due to N-H···N and O-H···O hydrogen bonds. In the crystal, the molecules are dimerized with each other due to pairs of N-H···O hydrogen bonds, forming an  $R_2^2(8)$  ring motif. O-H···O hydrogen bonds lead to the formation of a three-dimensional network.

#### **Related literature**

For a related structure, see: Tahir *et al.* (2012). For graph-set notation, see: Bernstein *et al.* (1995).



#### Experimental

Crystal data  $C_9H_{11}N_3O_3$   $M_r = 209.21$ Orthorhombic,  $Pca2_1$ a = 13.9945 (14) Å b = 5.0440 (4) Å

c = 27.280 (2) A
V = 1926.0 (3) Å <sup>3</sup>
Z = 8

Mo  $K\alpha$  radiation  $\mu = 0.11 \text{ mm}^{-1}$ 

#### Data collection

Bruker Kappa APEXII CCD diffractometer Absorption correction: multi-scan (SADABS; Bruker, 2005)  $T_{min} = 0.957, T_{max} = 0.966$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.056$ 275 parameters $wR(F^2) = 0.113$ H-atom parameters constrainedS = 0.98 $\Delta \rho_{max} = 0.22$  e Å<sup>-3</sup>1931 reflections $\Delta \rho_{min} = -0.25$  e Å<sup>-3</sup>

# Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$O2-H2A\cdots O1$	0.82	2.17	2.627 (6)	115
$O2-H2A\cdots O5^{1}$	0.82	2.34	3.108 (7)	156
$N2-H2B\cdots O6^{ii}$	0.86	2.11	2.923 (7)	158
$N3-H3A\cdots O6^{iii}$	0.86	2.16	2.987 (7)	162
$N3 - H3B \cdot \cdot \cdot N1$	0.86	2.31	2.674 (8)	106
$O5-H5A\cdots O4$	0.82	2.18	2.632 (6)	115
$N5-H5B\cdots O3^{iv}$	0.86	2.08	2.909 (7)	161
$N6-H6A\cdotsO3^{v}$	0.86	2.13	2.965 (7)	164
$N6-H6B\cdots N4$	0.86	2.32	2.677 (7)	105

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2364).

#### References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). Angew. Chem. Int. Ed. Engl. 34, 1555–1573.

Bruker (2005). SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2007). APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.

Farrugia, L. J. (1997). J. Appl. Cryst. 30, 565.

Farrugia, L. J. (1999). J. Appl. Cryst. 32, 837-838.

Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

Spek, A. L. (2009). Acta Cryst. D65, 148-155.

Tahir, M. N., Umar, M. N., Ali, A. & Shad, H. A. (2012). Acta Cryst. E68, 01724.

 $0.30 \times 0.16 \times 0.14 \text{ mm}$ 

8297 measured reflections

1931 independent reflections

1046 reflections with  $I > 2\sigma(I)$ 

T = 296 K

 $R_{\rm int} = 0.081$ 

# supplementary materials

Acta Cryst. (2012). E68, o2071 [doi:10.1107/S1600536812025299]

# (2E)-2-(4-Hydroxy-3-methoxybenzylidene)hydrazinecarboxamide

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## Comment

The title compound (I), (Fig. 1) has been synthesized as a derivative. Recently we have reported the crystal structure of (2E)-2-(3,4-dimethoxybenzylidene)hydrazinecarboxamide (Tahir *et al.*, 2012) which is related to the title compound. In (I), two molecules are present in the asymmetric unit, which differ slightly from each other geometrically. In one molecule, the parts of 4-hydroxy-3-methoxybenzaldehyde and hydrazinecarboxamide A (C1—C8/O1/O2) and B (N1/N2/C9/N3/O3), are almost planar with r.m.s. deviations of 0.0212 Å and 0.0066 Å, respectively. The dihedral angle between A/B is 16.57 (26)°. In the second molecule, the similar groups C (C10—C17/O4/O5) and D (N4/N5/C18/N6/O6) are also planar with r.m.s. deviations of 0.0346 Å and 0.0095 Å, respectively, and the dihedral angle between C/D is 9.74 (28)°. In both molecules two *S*(5) ring motifs (Bernstein *et al.*, 1995) are present due to H–bonding of N—H···N and O—H···O types (Table 1, Fig. 1). The molecules are dimerized with each other due to N—H···O type of H-bondings and form  $R_2^2(8)$  ring motifs (Table 1, Fig. 2). The molecules are stabilized in the form of three-dimensional polymeric network.

#### **Experimental**

Equimolar quantities of 4-hydroxy-3-methoxybenzaldehyde and hydrazinecarboxamide were refluxed in methanol along with few drops of acetic acid as catalyst for 45 min resulting in light orange solution. The solution was kept at room temperature which afforded light orange needles after few days.

## Refinement

In the absence of anomalous scattering all Friedel pairs were merged. The H-atoms were positioned geometrically (C–H = 0.93—0.96 Å, N—H = 0.86 Å, O—H = 0.82 Å) and refined as riding with  $U_{iso}(H) = xU_{eq}(C, N, O)$ , where x = 1.5 for hydroxy and methyl and x = 1.2 for other H-atoms.

## **Computing details**

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).



## Figure 1

View of the title compound with the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level.



## Figure 2

The partial packing (*PLATON*; Spek, 2009) which shows that molecules form ring motifs in three-dimensional polymeric network.

#### (2E)-2-(4-Hydroxy-3-methoxybenzylidene)hydrazinecarboxamide

#### Crystal data

C<sub>9</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>  $M_r = 209.21$ Orthorhombic,  $Pca2_1$ Hall symbol: P 2c -2ac a = 13.9945 (14) Å b = 5.0440 (4) Å c = 27.286 (2) Å V = 1926.0 (3) Å<sup>3</sup> Z = 8

#### Data collection

Bruker Kappa APEXII CCD	8297 measured reflections
diffractometer	1931 independent reflections
Radiation source: fine-focus sealed tube	1046 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\rm int} = 0.081$
Detector resolution: 8.00 pixels mm <sup>-1</sup>	$\theta_{\rm max} = 26.0^\circ, \ \theta_{\rm min} = 2.9^\circ$
$\omega$ scans	$h = -17 \rightarrow 17$
Absorption correction: multi-scan	$k = -3 \rightarrow 6$
(SADABS; Bruker, 2005)	$l = -33 \rightarrow 33$
$T_{\min} = 0.957, \ T_{\max} = 0.966$	
Refinement	

F(000) = 880

 $\theta = 1.8 - 26.0^{\circ}$  $\mu = 0.11 \text{ mm}^{-1}$ 

Needle, colorless

 $0.30 \times 0.16 \times 0.14 \text{ mm}$ 

T = 296 K

 $D_{\rm x} = 1.443 {\rm Mg} {\rm m}^{-3}$ 

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

Cell parameters from 2704 reflections

# Definement

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.039P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta \rho_{\rm max} = 0.22 \text{ e } \text{\AA}^{-3}$
$\Delta \rho_{\rm min} = -0.25 \text{ e } \text{\AA}^{-3}$

#### Special details

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement of  $F^2$  against ALL reflections. The weighted *R*-factor *wR* and goodness 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 threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating *R*-factors(gt) *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  $(Å^2)$ 

	x	у	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
01	0.1256 (3)	-0.4282 (10)	0.51673 (17)	0.051 (2)	
O2	0.3120 (3)	-0.4570 (10)	0.52664 (17)	0.0437 (19)	
03	-0.0668 (3)	0.7125 (10)	0.3095 (2)	0.0423 (16)	
N1	0.0730 (4)	0.3033 (11)	0.38554 (19)	0.035 (2)	
N2	0.0463 (3)	0.5085 (12)	0.3552 (2)	0.041 (2)	

N3 $-0.1032$ (4) $0.3268$ (12) $0.3479$ (2) $0.0481$ (2)C1 $0.1988$ (4) $0.0965$ (14) $0.4299$ (2) $0.031$ (3)C2 $0.1392$ (5) $-0.0745$ (13) $0.4553$ (3) $0.035$ (3)C3 $0.1755$ (4) $-0.2580$ (13) $0.4879$ (2) $0.031$ (2)C5 $0.3343$ (4) $-0.1063$ (13) $0.4703$ (2) $0.039$ (3)C6 $0.2995$ (4) $0.0792$ (13) $0.4384$ (2) $0.037$ (3)C7 $0.0252$ (4) $-0.4398$ (15) $0.5100$ (3) $0.049$ (3)C8 $0.1602$ (5) $0.2916$ (13) $0.3966$ (2) $0.032$ (2)C9 $-0.0445$ (4) $0.5255$ (14) $0.3362$ (2) $0.031$ (2)C4 $-0.199$ (3) $0.9504$ (9) $0.1503$ (17) $0.0413$ (16)C5 $-0.2032$ (3) $0.8811$ (10) $0.08760$ (18) $0.049$ (2)C6 $0.2021$ (3) $-0.1888$ (9) $0.31097$ (17) $0.0433$ (17)N4 $0.0595$ (3) $0.2198$ (10) $0.2364$ (2) $0.040$ (2)N5 $0.0884$ (4) $0.1926$ (10) $0.2705$ (2) $0.044$ (2)C10 $-0.0733$ (4) $0.4191$ (13) $0.1670$ (2) $0.029$ (2)C11 $-0.0188$ (4) $0.5961$ (13) $0.1670$ (2) $0.032$ (3)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (3)C15 $-0.1697$ (4) $0.3796$ (13) $0.1226$ (2) $0.033$ (2)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (2)C15 $-0.0697$ (4) </th <th></th> <th></th> <th></th> <th></th> <th></th>					
C1         0.1988 (4)         0.0965 (14)         0.4299 (2)         0.031 (3)           C2         0.1392 (5) $-0.0745$ (13)         0.4553 (3)         0.035 (3)           C3         0.1765 (4) $-0.2735$ (12)         0.4950 (2)         0.031 (2)           C5         0.3343 (4) $-0.1063$ (13)         0.4703 (2)         0.039 (3)           C6         0.2965 (4)         0.0792 (13)         0.4384 (2)         0.037 (3)           C7         0.0252 (4) $-0.4398$ (15)         0.5100 (3)         0.049 (3)           C8         0.1602 (5)         0.2916 (13)         0.3366 (2)         0.032 (2)           C9 $-0.0445$ (4)         0.5255 (14)         0.3362 (2)         0.031 (2)           C4 $-0.0199$ (3)         0.9504 (9)         0.10503 (17)         0.0443 (16)           C5 $-0.2032$ (3)         0.811 (10)         0.0870 (18)         0.037 (17)           N4         0.0595 (3)         0.2198 (10)         0.23612 (18)         0.037 (17)           N4         0.0595 (13)         0.1670 (2)         0.029 (2)         0.1613           C10 $-0.0733$ (4)         0.4199 (13)         0.1617 (2)         0.0235 (2)           C11 $-0.0636$	N3	-0.1032 (4)	0.3268 (12)	0.3479 (2)	0.048 (2)
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C4 $0.2739$ (5) $-0.2735$ (12) $0.4950$ (2) $0.031$ (2)C5 $0.3343$ (4) $-0.1063$ (13) $0.4703$ (2) $0.039$ (3)C6 $0.2955$ (4) $-0.792$ (13) $0.4384$ (2) $0.037$ (3)C7 $0.0252$ (4) $-0.4398$ (15) $0.5100$ (3) $0.049$ (3)C8 $0.1602$ (5) $0.2916$ (13) $0.3966$ (2) $0.031$ (2)C9 $-0.0445$ (4) $0.5255$ (14) $0.3562$ (2) $0.031$ (2)C4 $-0.0199$ (3) $0.9504$ (9) $0.10503$ (17) $0.0413$ (16)O5 $-0.2032$ (3) $0.8811$ (10) $0.8760$ (18) $0.049$ (2)O6 $0.2021$ (3) $-0.1888$ (9) $0.31097$ (17) $0.0430$ (17)N4 $0.0595$ (3) $0.2198$ (10) $0.27612$ (18) $0.0307$ (17)N5 $0.0884$ (4) $0.1926$ (10) $0.705$ (2) $0.044$ (2)C10 $-0.0733$ (4) $0.419$ (13) $0.1914$ (2) $0.031$ (2)C11 $-0.0188$ (4) $0.5961$ (13) $0.1570$ (2) $0.032$ (3)C12 $-0.0626$ (5) $0.7582$ (13) $0.1226$ (2) $0.033$ (2)C13 $-0.1603$ (4) $0.7257$ (13) $0.1226$ (2) $0.033$ (2)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (13) $0.388$ (3)C15 $-0.1697$ (4) $0.3764$ (13) $0.1890$ (2) $0.035$ (2)C16 $0.0808$ (4) $0.9841$ (14) $0.1099$ (3) $0.045$ (3)C17 $-0.0297$ (4) $0.2151$ (12) $0.2254$ (2) $0.033$ (2)H2 $0.0752$ </td <td>C3</td> <td>0.1765 (4)</td> <td>-0.2580 (13)</td> <td>0.4879 (2)</td> <td>0.031 (3)</td>	C3	0.1765 (4)	-0.2580 (13)	0.4879 (2)	0.031 (3)
C5 $0.3343$ (4) $-0.1063$ (13) $0.4703$ (2) $0.039$ (3)C6 $0.2965$ (4) $0.0792$ (13) $0.4384$ (2) $0.037$ (3)C7 $0.0252$ (4) $-0.4398$ (15) $0.5100$ (3) $0.0449$ (3)C8 $0.1602$ (5) $0.2916$ (13) $0.3966$ (2) $0.032$ (2)C9 $-0.0445$ (4) $0.5255$ (14) $0.3362$ (2) $0.031$ (2)O4 $-0.0199$ (3) $0.9504$ (9) $0.10503$ (17) $0.0443$ (16)O5 $-0.2032$ (3) $0.8811$ (10) $0.88760$ (18) $0.049$ (2)O6 $0.2021$ (3) $-0.1888$ (9) $0.31097$ (17) $0.0430$ (17)N4 $0.0595$ (3) $0.2198$ (10) $0.2268$ (2) $0.044$ (2)C10 $-0.0733$ (4) $0.189$ (11) $0.2668$ (2) $0.040$ (2)N5 $0.0884$ (4) $0.1189$ (11) $0.2668$ (2) $0.044$ (2)C11 $-0.0188$ (4) $0.1926$ (10) $0.2705$ (2) $0.031$ (2)C12 $-0.0626$ (5) $0.7582$ (13) $0.1326$ (2) $0.033$ (2)C13 $-0.1603$ (4) $0.7257$ (13) $0.1226$ (2) $0.033$ (2)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (3)C15 $-0.1697$ (4) $0.3796$ (13) $0.1809$ (2) $0.035$ (2)C16 $0.0808$ (4) $0.9841$ (14) $0.1099$ (3) $0.0444$ (3)C15 $-0.1697$ (4) $0.2757$ (1) $0.2544$ (2) $0.033$ (2)C16 $0.0808$ (4) $0.9841$ (14) $0.1099$ (3) $0.0424^*$ L2 $0.07552$ <td>C4</td> <td>0.2739 (5)</td> <td>-0.2735 (12)</td> <td>0.4950 (2)</td> <td>0.031 (2)</td>	C4	0.2739 (5)	-0.2735 (12)	0.4950 (2)	0.031 (2)
C6 $0.2965$ (4) $0.0792$ (13) $0.4384$ (2) $0.037$ (3)C7 $0.0252$ (4) $-0.4398$ (15) $0.5100$ (3) $0.049$ (3)C8 $0.1602$ (5) $0.2916$ (13) $0.3966$ (2) $0.031$ (2)C9 $-0.0445$ (4) $0.5255$ (14) $0.3362$ (2) $0.031$ (2)O4 $-0.0199$ (3) $0.9504$ (9) $0.10503$ (17) $0.0413$ (16)O5 $-0.2032$ (3) $0.8811$ (10) $0.2057$ (18) $0.0490$ (17)N4 $0.0595$ (3) $0.2198$ (10) $0.23612$ (18) $0.0307$ (17)N5 $0.0884$ (4) $0.11926$ (10) $0.705$ (2) $0.0444$ (2)C10 $-0.0733$ (4) $0.4019$ (13) $0.1914$ (2) $0.031$ (2)C11 $-0.0188$ (4) $0.5961$ (13) $0.1570$ (2) $0.029$ (2)C12 $-0.0626$ (5) $0.7582$ (13) $0.1226$ (2) $0.032$ (3)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (3)C15 $-0.1697$ (4) $0.3796$ (13) $0.1226$ (2) $0.033$ (2)C16 $0.0808$ (4) $0.9841$ (14) $0.1099$ (3) $0.0445$ (3)C17 $-0.0297$ (4) $0.2151$ (12) $0.2254$ (2) $0.033$ (2)C18 $0.1785$ (5) $0.0009$ (15) $0.24545$ (2) $0.033$ (2)C19 $0.03772$ $0.2684$ $0.47685$ $0.0490^*$ H20 $0.03772$ $0.22442$ $0.34765$ $0.490^*$ H31 $-0.06371$ $0.254591$ $0.36668$ $0.0569^*$ H33 $-0.06372$ $0.34795$ $0.$	C5	0.3343 (4)	-0.1063 (13)	0.4703 (2)	0.039 (3)
C7 $0.0252 (4)$ $-0.4398 (15)$ $0.5100 (3)$ $0.049 (3)$ C8 $0.1602 (5)$ $0.2916 (13)$ $0.3966 (2)$ $0.032 (2)$ C9 $-0.0445 (4)$ $0.5255 (14)$ $0.3562 (2)$ $0.031 (2)$ O4 $-0.0199 (3)$ $0.9504 (9)$ $0.10503 (17)$ $0.0413 (16)$ O5 $-0.2032 (3)$ $0.8811 (10)$ $0.08760 (18)$ $0.049 (2)$ O6 $0.2021 (3)$ $-0.1888 (9)$ $0.31097 (17)$ $0.0430 (17)$ N4 $0.0595 (3)$ $0.2198 (10)$ $0.23612 (18)$ $0.0307 (17)$ N5 $0.0884 (4)$ $0.0192 (10)$ $0.2705 (2)$ $0.044 (2)$ C10 $-0.0733 (4)$ $0.4019 (13)$ $0.1914 (2)$ $0.031 (2)$ C11 $-0.082 (5)$ $0.7582 (13)$ $0.1226 (2)$ $0.030 (2)$ C12 $-0.0626 (5)$ $0.7582 (13)$ $0.1226 (2)$ $0.030 (2)$ C13 $-0.1603 (4)$ $0.7257 (13)$ $0.1226 (2)$ $0.033 (2)$ C14 $-0.2137 (5)$ $0.5398 (14)$ $0.1471 (3)$ $0.388 (3)$ C15 $-0.1697 (4)$ $0.3796 (13)$ $0.1809 (2)$ $0.035 (2)$ C16 $0.0808 (4)$ $0.9841 (14)$ $0.1991 (3)$ $0.045 (3)$ C17 $-0.0297 (4)$ $0.2151 (12)$ $0.2254 (2)$ $0.033 (2)$ L12 $0.0755 (5)$ $0.32439$ $0.33656$ $0.0569^*$ H3A $-0.16059$ $0.32439$ $0.33656$ $0.0569^*$ H3B $-0.0872$ $0.2151 (12)$ $0.2244$ $0.0444^*$ H2A $0.2264 (2)$ $0.33740$ <td>C6</td> <td>0.2965 (4)</td> <td>0.0792 (13)</td> <td>0.4384 (2)</td> <td>0.037 (3)</td>	C6	0.2965 (4)	0.0792 (13)	0.4384 (2)	0.037 (3)
C8 $0.1602$ (5) $0.2916$ (13) $0.3966$ (2) $0.032$ (2)C9 $-0.0445$ (4) $0.5255$ (14) $0.3362$ (2) $0.031$ (2)O4 $-0.0199$ (3) $0.9504$ (9) $0.10503$ (17) $0.0413$ (16)O5 $-0.2022$ (3) $0.8811$ (10) $0.08760$ (18) $0.0499$ (2)O6 $0.2021$ (3) $-0.1888$ (9) $0.31097$ (17) $0.0430$ (17)N4 $0.0595$ (3) $0.2198$ (10) $0.23612$ (18) $0.0307$ (17)N5 $0.0884$ (4) $0.11926$ (10) $0.2705$ (2) $0.044$ (2)C10 $-0.0733$ (4) $0.4019$ (13) $0.1914$ (2) $0.031$ (2)C11 $-0.0188$ (4) $0.5961$ (13) $0.1670$ (2) $0.032$ (3)C12 $-0.6626$ (5) $0.7582$ (13) $0.1226$ (2) $0.030$ (2)C13 $-0.1603$ (4) $0.7257$ (13) $0.1226$ (2) $0.033$ (3)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (3)C15 $-0.1697$ (4) $0.2151$ (12) $0.2254$ (2) $0.030$ (2)C16 $0.808$ (4) $0.9841$ (14) $0.1099$ (3) $0.045$ (3)C17 $-0.0297$ (4) $0.2151$ (12) $0.2254$ (2) $0.030$ (2)C18 $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2)H2 $0.0757$ $0.26892$ $0.34795$ $0.0490^*$ H3B $-0.06370$ $0.2174$ $0.36668$ $0.569^*$ H3B $-0.0877$ $0.25066$ $0.53213$ $0.0593^*$ H7B $-0.00207$ $-0.26864$ $0.$	C7	0.0252 (4)	-0.4398 (15)	0.5100 (3)	0.049 (3)
C9 $-0.0445$ (4) $0.5255$ (14) $0.3362$ (2) $0.031$ (2)O4 $-0.0199$ (3) $0.9504$ (9) $0.10503$ (17) $0.0413$ (16)O5 $-0.2032$ (3) $0.8811$ (10) $0.08760$ (18) $0.049$ (2)O6 $0.2021$ (3) $-0.1888$ (9) $0.31097$ (17) $0.0430$ (17)N4 $0.0595$ (3) $0.2198$ (10) $0.23612$ (18) $0.0307$ (17)N5 $0.0884$ (4) $0.11926$ (10) $0.2705$ (2) $0.044$ (2)C10 $-0.0733$ (4) $0.4019$ (13) $0.1914$ (2) $0.031$ (2)C11 $-0.0188$ (4) $0.5961$ (13) $0.1670$ (2) $0.022$ (3)C12 $-0.0626$ (5) $0.7252$ (13) $0.1226$ (2) $0.032$ (3)C13 $-0.1603$ (4) $0.7257$ (13) $0.1226$ (2) $0.033$ (2)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (3)C15 $-0.1697$ (4) $0.3766$ (13) $0.1809$ (2) $0.035$ (2)C16 $0.0080$ (4) $0.9841$ (14) $0.1099$ (3) $0.045$ (3)C17 $-0.0297$ (4) $0.2151$ (12) $0.2254$ (2) $0.030$ (2)C18 $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2)C18 $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2)H2A $0.26884$ $-0.54591$ $0.35666$ $0.0569*$ H3B $-0.08372$ $0.2124$ $0.34458$ $0.4424*$ H2A $0.26884$ $-0.54591$ $0.35666$ $0.0569*$ H3B $-0.00207$ $-0.26864$	C8	0.1602 (5)	0.2916 (13)	0.3966 (2)	0.032 (2)
$04$ $-0.0199$ (3) $0.9504$ (9) $0.10503$ (17) $0.0413$ (16) $05$ $-0.2032$ (3) $0.8811$ (10) $0.08760$ (18) $0.049$ (2) $06$ $0.2021$ (3) $-0.1888$ (9) $0.31097$ (17) $0.0430$ (17) $N4$ $0.0585$ (3) $0.2198$ (10) $0.23612$ (18) $0.0307$ (17) $N5$ $0.0884$ (4) $0.0189$ (11) $0.2668$ (2) $0.040$ (2) $N6$ $0.2384$ (4) $0.0189$ (11) $0.2668$ (2) $0.044$ (2) $C10$ $-0.0733$ (4) $0.4019$ (13) $0.1914$ (2) $0.031$ (2) $C11$ $-0.0188$ (4) $0.5961$ (13) $0.1670$ (2) $0.030$ (2) $C13$ $-0.1603$ (4) $0.7257$ (13) $0.1226$ (2) $0.033$ (3) $C14$ $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (3) $C15$ $-0.1697$ (4) $0.3796$ (13) $0.1809$ (2) $0.035$ (2) $C16$ $0.0808$ (4) $0.9841$ (14) $0.1099$ (3) $0.045$ (3) $C17$ $-0.0297$ (4) $0.2151$ (12) $0.2254$ (2) $0.033$ (2) $C18$ $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2) $H2A$ $0.26884$ $-0.54591$ $0.53860$ $0.0649^*$ $H2B$ $0.08747$ $0.62892$ $0.34795$ $0.0490^*$ $H3B$ $-0.08372$ $0.20124$ $0.36668$ $0.0569^*$ $H3B$ $-0.08372$ $0.2124$ $0.36668$ $0.0593^*$ $H7B$ $-0.0207$ $-0.26864$ $0.51642$ $0.0593^*$ $H7B$ $-0.0027$	C9	-0.0445 (4)	0.5255 (14)	0.3362 (2)	0.031 (2)
O5 $-0.2032$ (3) $0.8811$ (10) $0.08760$ (18) $0.049$ (2)O6 $0.2021$ (3) $-0.1888$ (9) $0.31097$ (17) $0.0430$ (17)N4 $0.0595$ (3) $0.2198$ (10) $0.23612$ (18) $0.0307$ (17)N5 $0.0884$ (4) $0.0189$ (11) $0.2668$ (2) $0.040$ (2)N6 $0.2384$ (4) $0.1926$ (10) $0.2705$ (2) $0.044$ (2)C10 $-0.0733$ (4) $0.4019$ (13) $0.1914$ (2) $0.031$ (2)C11 $-0.0188$ (4) $0.5961$ (13) $0.1670$ (2) $0.032$ (3)C12 $-0.0626$ (5) $0.7582$ (13) $0.1326$ (2) $0.033$ (2)C13 $-0.1603$ (4) $0.7257$ (13) $0.1226$ (2) $0.033$ (3)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (3)C15 $-0.1697$ (4) $0.3796$ (13) $0.1899$ (2) $0.035$ (2)C16 $0.0808$ (4) $0.99841$ (14) $0.1999$ (3) $0.045$ (3)C17 $-0.0297$ (4) $0.2151$ (12) $0.2254$ (2) $0.033$ (2)C18 $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2)C18 $0.7825$ $-0.66591$ $0.45048$ $0.0424*$ H2A $0.26884$ $-0.54591$ $0.53860$ $0.6649*$ H2B $0.08747$ $0.62892$ $0.34795$ $0.0490*$ H3A $-0.1695$ $0.32439$ $0.33656$ $0.0569*$ H3B $-0.08372$ $0.20124$ $0.36668$ $0.0593*$ H7B $-0.00207$ $-0.26864$ $0.51642$ $0.0593*$ <	O4	-0.0199(3)	0.9504 (9)	0.10503 (17)	0.0413 (16)
O6 $0.2021$ (3) $-0.1888$ (9) $0.31097$ (17) $0.0430$ (17)N4 $0.0595$ (3) $0.2198$ (10) $0.23612$ (18) $0.0307$ (17)N5 $0.0884$ (4) $0.189$ (11) $0.2668$ (2) $0.044$ (2)C10 $-0.0733$ (4) $0.1926$ (10) $0.2705$ (2) $0.044$ (2)C11 $-0.0188$ (4) $0.5961$ (13) $0.1914$ (2) $0.030$ (2)C12 $-0.0626$ (5) $0.7582$ (13) $0.1226$ (2) $0.032$ (3)C13 $-0.1603$ (4) $0.7257$ (13) $0.1226$ (2) $0.032$ (3)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (3)C15 $-0.1697$ (4) $0.3796$ (13) $0.1809$ (2) $0.035$ (2)C16 $0.0808$ (4) $0.9841$ (14) $0.1999$ (3) $0.045$ (3)C17 $-0.0297$ (4) $0.2151$ (12) $0.2254$ (2) $0.033$ (2)C18 $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2)H2 $0.07352$ $-0.06591$ $0.45048$ $0.0424*$ H2A $0.26884$ $-0.54591$ $0.53860$ $0.669*$ H3B $-0.08372$ $0.20124$ $0.36668$ $0.0569*$ H3B $-0.08372$ $0.20124$ $0.36668$ $0.0593*$ H7M $0.01136$ $-0.49086$ $0.47685$ $0.0593*$ H7B $-0.00207$ $-0.26844$ $0.51642$ $0.0593*$ H7B $-0.00207$ $-0.26864$ $0.51642$ $0.0593*$ H7B $-0.00207$ $-0.26864$ $0.17385$ $0.0593*$ H7B	05	-0.2032 (3)	0.8811 (10)	0.08760 (18)	0.049 (2)
N4 $0.0595$ (3) $0.2198$ (10) $0.23612$ (18) $0.0307$ (17)N5 $0.0884$ (4) $0.0189$ (11) $0.2668$ (2) $0.040$ (2)N6 $0.2384$ (4) $0.1926$ (10) $0.2705$ (2) $0.044$ (2)C10 $-0.0733$ (4) $0.4019$ (13) $0.1914$ (2) $0.031$ (2)C11 $-0.0188$ (4) $0.5961$ (13) $0.1670$ (2) $0.029$ (2)C12 $-0.0626$ (5) $0.7582$ (13) $0.1226$ (2) $0.030$ (2)C13 $-0.1603$ (4) $0.7257$ (13) $0.1226$ (2) $0.033$ (3)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (3)C15 $-0.1697$ (4) $0.3796$ (13) $0.1809$ (2) $0.035$ (2)C16 $0.0808$ (4) $0.9841$ (14) $0.1099$ (3) $0.045$ (3)C17 $-0.0297$ (4) $0.2151$ (12) $0.2245$ (2) $0.033$ (2)C18 $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2)C18 $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2)L2 $0.07352$ $-0.6591$ $0.45048$ $0.0424*$ H2A $0.26884$ $-0.54591$ $0.53860$ $0.0669*$ H3B $-0.08372$ $0.20124$ $0.36668$ $0.0559*$ H3B $-0.0207$ $-0.26864$ $0.51642$ $0.0593*$ H7A $0.01136$ $-0.49086$ $0.47685$ $0.0393*$ H7B $-0.00207$ $-0.26864$ $0.51642$ $0.0593*$ H7A $0.0207$ $-0.26864$ $0.51642$ $0.0593*$	O6	0.2021 (3)	-0.1888 (9)	0.31097 (17)	0.0430 (17)
N5         0.0884 (4)         0.0189 (11)         0.2668 (2)         0.040 (2)           N6         0.2384 (4)         0.1926 (10)         0.2705 (2)         0.044 (2)           C10         -0.0733 (4)         0.4019 (13)         0.1914 (2)         0.031 (2)           C11         -0.0188 (4)         0.5961 (13)         0.1670 (2)         0.029 (2)           C12         -0.0626 (5)         0.7582 (13)         0.1226 (2)         0.033 (2)           C14         -0.2137 (5)         0.5398 (14)         0.1471 (3)         0.038 (3)           C15         -0.1697 (4)         0.3796 (13)         0.1809 (2)         0.035 (2)           C16         0.0808 (4)         0.9841 (14)         0.1471 (3)         0.038 (3)           C17         -0.0297 (4)         0.2151 (12)         0.2254 (2)         0.033 (2)           C18         0.1785 (5)         0.0009 (15)         0.2845 (2)         0.033 (2)           H2         0.07352         -0.06591         0.45048         0.0424*           H2A         0.26884         -0.54591         0.35860         0.0649*           H2B         0.08747         0.62892         0.34795         0.0440*           H3A         -0.16059         0.32439         0.3365	N4	0.0595 (3)	0.2198 (10)	0.23612 (18)	0.0307 (17)
N6 $0.2384$ (4) $0.1926$ (10) $0.2705$ (2) $0.044$ (2)C10 $-0.0733$ (4) $0.4019$ (13) $0.1914$ (2) $0.031$ (2)C11 $-0.0188$ (4) $0.5961$ (13) $0.1670$ (2) $0.029$ (2)C12 $-0.0626$ (5) $0.7582$ (13) $0.1326$ (2) $0.030$ (2)C13 $-0.1603$ (4) $0.7257$ (13) $0.1226$ (2) $0.032$ (3)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (3)C15 $-0.1697$ (4) $0.3796$ (13) $0.1809$ (2) $0.035$ (2)C16 $0.0808$ (4) $0.9841$ (14) $0.1099$ (3) $0.045$ (3)C17 $-0.0297$ (4) $0.2151$ (12) $0.2254$ (2) $0.030$ (2)C18 $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2)H2 $0.07352$ $-0.06591$ $0.45048$ $0.0424*$ H2A $0.26884$ $-0.54591$ $0.53860$ $0.669*$ H3B $-0.08372$ $0.20124$ $0.36668$ $0.0569*$ H3B $-0.08372$ $0.20124$ $0.36668$ $0.0569*$ H5 $0.40001$ $-0.1747$ $0.47486$ $0.0444*$ H6 $0.33740$ $0.19515$ $0.42224$ $0.0444*$ H7A $0.0136$ $-0.49086$ $0.47685$ $0.0593*$ H7B $-0.00207$ $-0.26864$ $0.51642$ $0.0593*$ H7A $0.0159$ $-0.56760$ $0.53213$ $0.0593*$ H7B $-0.16623$ $0.99847$ $0.07909$ $0.729*$ H5B $0.41433$ $0.38265$ </td <td>N5</td> <td>0.0884 (4)</td> <td>0.0189 (11)</td> <td>0.2668 (2)</td> <td>0.040 (2)</td>	N5	0.0884 (4)	0.0189 (11)	0.2668 (2)	0.040 (2)
C10 $-0.0733$ (4) $0.4019$ (13) $0.1914$ (2) $0.031$ (2)C11 $-0.0188$ (4) $0.5961$ (13) $0.1670$ (2) $0.029$ (2)C12 $-0.0626$ (5) $0.7582$ (13) $0.1326$ (2) $0.030$ (2)C13 $-0.1603$ (4) $0.7257$ (13) $0.1226$ (2) $0.032$ (3)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (3)C15 $-0.1697$ (4) $0.3796$ (13) $0.1809$ (2) $0.035$ (2)C16 $0.0808$ (4) $0.9841$ (14) $0.1099$ (3) $0.045$ (3)C17 $-0.0297$ (4) $0.2151$ (12) $0.2254$ (2) $0.033$ (2)C18 $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2)C18 $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2)H2 $0.07352$ $-0.06591$ $0.45048$ $0.0424*$ H2A $0.26884$ $-0.54591$ $0.53860$ $0.0649*$ H2B $0.08747$ $0.62892$ $0.34795$ $0.0490*$ H3A $-0.16059$ $0.32439$ $0.36566$ $0.0569*$ H5 $0.40001$ $-0.11747$ $0.47486$ $0.0464*$ H6 $0.33740$ $0.19515$ $0.42224$ $0.0444*$ H7A $0.01136$ $-0.49086$ $0.47685$ $0.0593*$ H7B $-0.0207$ $-0.26864$ $0.51642$ $0.593*$ H7B $-0.0207$ $-0.26864$ $0.51642$ $0.593*$ H7A $0.01136$ $-0.49086$ $0.47685$ $0.03534*$ H5A $-0.16623$ $0.9984$	N6	0.2384 (4)	0.1926 (10)	0.2705 (2)	0.044 (2)
C11         -0.0188 (4)         0.5961 (13)         0.1670 (2)         0.029 (2)           C12         -0.0626 (5)         0.7582 (13)         0.1326 (2)         0.030 (2)           C13         -0.1603 (4)         0.7257 (13)         0.1226 (2)         0.038 (3)           C14         -0.2137 (5)         0.5398 (14)         0.1471 (3)         0.038 (3)           C15         -0.1697 (4)         0.3796 (13)         0.1809 (2)         0.035 (2)           C16         0.8088 (4)         0.9841 (14)         0.1099 (3)         0.045 (3)           C17         -0.0297 (4)         0.2151 (12)         0.2254 (2)         0.030 (2)           C18         0.1785 (5)         0.0009 (15)         0.2845 (2)         0.033 (2)           H2         0.07352         -0.06591         0.45048         0.0424*           H2A         0.26884         -0.65891         0.53860         0.0649*           H2B         0.08747         0.62892         0.34795         0.0490*           H3A         -0.16059         0.32439         0.36668         0.0569*           H3B         -0.08372         0.20124         0.36668         0.0593*           H7B         0.00207         -0.26864         0.51642         0	C10	-0.0733 (4)	0.4019 (13)	0.1914 (2)	0.031 (2)
C12 $-0.0626 (5)$ $0.7582 (13)$ $0.1326 (2)$ $0.030 (2)$ C13 $-0.1603 (4)$ $0.7257 (13)$ $0.1226 (2)$ $0.032 (3)$ C14 $-0.2137 (5)$ $0.5398 (14)$ $0.1471 (3)$ $0.038 (3)$ C15 $-0.1697 (4)$ $0.3796 (13)$ $0.1809 (2)$ $0.035 (2)$ C16 $0.0808 (4)$ $0.9841 (14)$ $0.1099 (3)$ $0.045 (3)$ C17 $-0.0297 (4)$ $0.2151 (12)$ $0.2254 (2)$ $0.030 (2)$ C18 $0.1785 (5)$ $0.0009 (15)$ $0.2845 (2)$ $0.033 (2)$ H2 $0.07352$ $-0.06591$ $0.45048$ $0.0424*$ H2A $0.26884$ $-0.54591$ $0.53860$ $0.0649*$ H2B $0.08747$ $0.62892$ $0.34795$ $0.0490*$ H3A $-0.16059$ $0.32439$ $0.33656$ $0.0569*$ H3B $-0.08372$ $0.20124$ $0.36668$ $0.0569*$ H5 $0.40001$ $-0.11747$ $0.47486$ $0.0444*$ H6 $0.33740$ $0.19515$ $0.42224$ $0.0444*$ H7A $0.01136$ $-0.49086$ $0.47685$ $0.0593*$ H7B $-0.00207$ $-0.26864$ $0.51642$ $0.0593*$ H7C $-0.00159$ $-0.56760$ $0.53213$ $0.0593*$ H8 $0.20166$ $0.41433$ $0.38265$ $0.0377*$ H5A $-0.16623$ $0.99847$ $0.7998$ $0.0534*$ H6B $0.21835$ $0.31947$ $0.25217$ $0.0534*$ H6B $0.22777$ $0.52269$ $0.14088$ $0.0458*$	C11	-0.0188 (4)	0.5961 (13)	0.1670 (2)	0.029 (2)
C13 $-0.1603$ (4) $0.7257$ (13) $0.1226$ (2) $0.032$ (3)C14 $-0.2137$ (5) $0.5398$ (14) $0.1471$ (3) $0.038$ (3)C15 $-0.1697$ (4) $0.3796$ (13) $0.1809$ (2) $0.035$ (2)C16 $0.0808$ (4) $0.9841$ (14) $0.1099$ (3) $0.045$ (3)C17 $-0.0297$ (4) $0.2151$ (12) $0.2254$ (2) $0.030$ (2)C18 $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2)H2 $0.07352$ $-0.06591$ $0.45048$ $0.0424^*$ H2A $0.26884$ $-0.54591$ $0.53860$ $0.0649^*$ H3A $-0.16059$ $0.32439$ $0.33656$ $0.0569^*$ H3B $-0.08372$ $0.20124$ $0.36668$ $0.0569^*$ H5 $0.40001$ $-0.11747$ $0.47486$ $0.0464^*$ H6 $0.33740$ $0.19515$ $0.42224$ $0.0444^*$ H7A $0.01136$ $-0.49086$ $0.47685$ $0.0593^*$ H7B $-0.00207$ $-0.26864$ $0.51642$ $0.0593^*$ H7A $0.01159$ $-0.56760$ $0.53213$ $0.0593^*$ H7B $-0.0207$ $-0.26864$ $0.51642$ $0.0377^*$ H5A $-0.16623$ $0.99847$ $0.07909$ $0.729^*$ H5B $0.04750$ $-0.10020$ $0.27510$ $0.0479^*$ H6A $0.29709$ $0.18908$ $0.27988$ $0.05534^*$ H11 $0.04595$ $0.61546$ $0.17385$ $0.0351^*$ H14 $-0.27877$ $0.52269$ $0.14088$ $0.$	C12	-0.0626 (5)	0.7582 (13)	0.1326 (2)	0.030 (2)
C14         -0.2137 (5)         0.5398 (14)         0.1471 (3)         0.038 (3)           C15         -0.1697 (4)         0.3796 (13)         0.1809 (2)         0.035 (2)           C16         0.0808 (4)         0.9841 (14)         0.1099 (3)         0.045 (3)           C17         -0.0297 (4)         0.2151 (12)         0.2254 (2)         0.030 (2)           C18         0.1785 (5)         0.0009 (15)         0.2845 (2)         0.033 (2)           H2         0.07352         -0.06591         0.45048         0.0424*           H2A         0.26884         -0.54591         0.53860         0.0649*           H2B         0.08747         0.62892         0.34795         0.0490*           H3A         -0.16059         0.32439         0.33656         0.0569*           H3B         -0.08372         0.20124         0.36668         0.0569*           H5         0.40001         -0.11747         0.47486         0.0444*           H7A         0.01136         -0.49086         0.47685         0.0593*           H7B         -0.00207         -0.26864         0.51642         0.0593*           H7C         -0.00159         -0.56760         0.53213         0.0593*	C13	-0.1603 (4)	0.7257 (13)	0.1226 (2)	0.032 (3)
C15 $-0.1697 (4)$ $0.3796 (13)$ $0.1809 (2)$ $0.035 (2)$ C16 $0.0808 (4)$ $0.9841 (14)$ $0.1099 (3)$ $0.045 (3)$ C17 $-0.0297 (4)$ $0.2151 (12)$ $0.2254 (2)$ $0.030 (2)$ C18 $0.1785 (5)$ $0.0009 (15)$ $0.2845 (2)$ $0.033 (2)$ H2 $0.07352$ $-0.06591$ $0.45048$ $0.0424*$ H2A $0.26884$ $-0.54591$ $0.53860$ $0.0649*$ H3A $-0.16059$ $0.32439$ $0.33656$ $0.0569*$ H3B $-0.08372$ $0.20124$ $0.36668$ $0.0569*$ H5 $0.40001$ $-0.11747$ $0.47486$ $0.0444*$ H6 $0.33740$ $0.19515$ $0.42224$ $0.0444*$ H7A $0.01136$ $-0.49086$ $0.47685$ $0.0593*$ H7B $-0.00207$ $-0.26864$ $0.51642$ $0.0593*$ H7C $-0.00159$ $-0.56760$ $0.53213$ $0.0593*$ H8 $0.20166$ $0.41433$ $0.38265$ $0.0377*$ H5A $-0.16c23$ $0.99847$ $0.07909$ $0.0729*$ H5B $0.4750$ $-0.18020$ $0.27510$ $0.0448*$ H6B $0.21835$ $0.31947$ $0.25217$ $0.6534*$ H11 $0.04595$ $0.61546$ $0.17385$ $0.0351*$ H14 $-0.27877$ $0.52269$ $0.14088$ $0.0458*$ H15 $-0.20577$ $0.25249$ $0.19730$ $0.0421*$ H16A $0.11246$ $0.81983$ $0.10266$ $0.0675*$ H16B $0.$	C14	-0.2137 (5)	0.5398 (14)	0.1471 (3)	0.038 (3)
C16         0.808 (4)         0.9841 (14)         0.1099 (3)         0.045 (3)           C17         -0.0297 (4)         0.2151 (12)         0.2254 (2)         0.030 (2)           C18         0.1785 (5)         0.0009 (15)         0.2845 (2)         0.033 (2)           H2         0.07352         -0.06591         0.45048         0.0424*           H2A         0.26884         -0.54591         0.53860         0.0649*           H2B         0.08747         0.62892         0.34795         0.0490*           H3A         -0.16059         0.32439         0.33656         0.0569*           H3B         -0.08372         0.20124         0.36668         0.0464*           H6         0.33740         0.19515         0.42224         0.0444*           H7A         0.01136         -0.49086         0.47685         0.0593*           H7B         -0.00207         -0.26864         0.51642         0.0593*           H7C         -0.00159         -0.56760         0.53213         0.0593*           H8         0.20166         0.41433         0.38265         0.0377*           H5B         0.04750         -0.10020         0.27510         0.0479*           H6A <td< td=""><td>C15</td><td>-0.1697 (4)</td><td>0.3796 (13)</td><td>0.1809 (2)</td><td>0.035 (2)</td></td<>	C15	-0.1697 (4)	0.3796 (13)	0.1809 (2)	0.035 (2)
C17         -0.0297 (4)         0.2151 (12)         0.2254 (2)         0.030 (2)           C18         0.1785 (5)         0.0009 (15)         0.2845 (2)         0.033 (2)           H2         0.07352         -0.06591         0.45048         0.0424*           H2A         0.26884         -0.54591         0.53860         0.0649*           H2B         0.08747         0.62892         0.34795         0.0490*           H3A         -0.16059         0.32439         0.33656         0.0569*           H3B         -0.08372         0.20124         0.36668         0.0644*           H6         0.33740         0.19515         0.42224         0.0444*           H7A         0.01136         -0.49086         0.47685         0.0593*           H7B         -0.00207         -0.26864         0.51642         0.0593*           H7C         -0.00159         -0.56760         0.53213         0.0593*           H8         0.20166         0.41433         0.38265         0.0377*           H5B         0.04750         -0.10020         0.27510         0.0479*           H6A         0.29709         0.18908         0.27988         0.0534*           H6B         0.21835 <td>C16</td> <td>0.0808 (4)</td> <td>0.9841 (14)</td> <td>0.1099 (3)</td> <td>0.045 (3)</td>	C16	0.0808 (4)	0.9841 (14)	0.1099 (3)	0.045 (3)
C18 $0.1785$ (5) $0.0009$ (15) $0.2845$ (2) $0.033$ (2)H2 $0.07352$ $-0.06591$ $0.45048$ $0.0424*$ H2A $0.26884$ $-0.54591$ $0.53860$ $0.0649*$ H2B $0.08747$ $0.62892$ $0.34795$ $0.0490*$ H3A $-0.16059$ $0.32439$ $0.33656$ $0.0569*$ H3B $-0.08372$ $0.20124$ $0.36668$ $0.0569*$ H5 $0.40001$ $-0.11747$ $0.47486$ $0.0444*$ H6 $0.33740$ $0.19515$ $0.42224$ $0.0444*$ H7A $0.01136$ $-0.49086$ $0.47685$ $0.0593*$ H7B $-0.00207$ $-0.26864$ $0.51642$ $0.0593*$ H7C $-0.00159$ $-0.56760$ $0.53213$ $0.0593*$ H8 $0.20166$ $0.41433$ $0.38265$ $0.0377*$ H5A $-0.16623$ $0.99847$ $0.07909$ $0.0729*$ H5B $0.04750$ $-0.10020$ $0.27510$ $0.0479*$ H6A $0.29709$ $0.18908$ $0.27988$ $0.0534*$ H11 $0.04595$ $0.61546$ $0.17385$ $0.0351*$ H14 $-0.27877$ $0.52269$ $0.14088$ $0.0458*$ H15 $-0.20577$ $0.25249$ $0.19730$ $0.0421*$ H16A $0.11246$ $0.81983$ $0.10266$ $0.0675*$ H16B $0.09561$ $1.03701$ $0.14284$ $0.0675*$ H16C $0.10226$ $1.11826$ $0.08749$ $0.0675*$ H16C $0.10226$ $1.11826$ $0$	C17	-0.0297 (4)	0.2151 (12)	0.2254 (2)	0.030 (2)
H2 $0.07352$ $-0.06591$ $0.45048$ $0.0424*$ H2A $0.26884$ $-0.54591$ $0.53860$ $0.0649*$ H2B $0.08747$ $0.62892$ $0.34795$ $0.0490*$ H3A $-0.16059$ $0.32439$ $0.33656$ $0.0569*$ H3B $-0.08372$ $0.20124$ $0.36668$ $0.0569*$ H5 $0.40001$ $-0.11747$ $0.47486$ $0.0464*$ H6 $0.33740$ $0.19515$ $0.42224$ $0.0444*$ H7A $0.01136$ $-0.49086$ $0.47685$ $0.0593*$ H7B $-0.00207$ $-0.26864$ $0.51642$ $0.0593*$ H7C $-0.00159$ $-0.56760$ $0.53213$ $0.0593*$ H8 $0.20166$ $0.41433$ $0.38265$ $0.0377*$ H5A $-0.16623$ $0.99847$ $0.07909$ $0.0729*$ H5B $0.04750$ $-0.10020$ $0.27510$ $0.0479*$ H6A $0.29709$ $0.18908$ $0.27988$ $0.0534*$ H6B $0.21835$ $0.31947$ $0.25217$ $0.0534*$ H11 $0.04595$ $0.61546$ $0.17385$ $0.0351*$ H14 $-0.27877$ $0.52269$ $0.14088$ $0.0458*$ H15 $-0.20577$ $0.25249$ $0.19730$ $0.0421*$ H16A $0.11246$ $0.81983$ $0.10266$ $0.0675*$ H16B $0.09561$ $1.03701$ $0.14284$ $0.0675*$ H16C $0.10226$ $1.11826$ $0.08749$ $0.075*$ H17 $-0.06819$ $0.08711$ $0.23996$ <	C18	0.1785 (5)	0.0009 (15)	0.2845 (2)	0.033 (2)
H2A0.26884-0.545910.538600.0649*H2B0.087470.628920.347950.0490*H3A-0.160590.324390.336560.0569*H3B-0.083720.201240.366680.0669*H50.40001-0.117470.474860.0464*H60.337400.195150.422240.0444*H7A0.01136-0.490860.476850.0593*H7B-0.00207-0.268640.516420.0593*H7C-0.00159-0.567600.532130.0593*H80.201660.414330.382650.0377*H5A-0.166230.998470.079090.0729*H5B0.04750-0.100200.275100.0479*H6A0.297090.189080.279880.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H2	0.07352	-0.06591	0.45048	0.0424*
H2B0.087470.628920.347950.0490*H3A-0.160590.324390.336560.0569*H3B-0.083720.201240.366680.0569*H50.40001-0.117470.474860.0464*H60.337400.195150.422240.0444*H7A0.01136-0.490860.476850.0593*H7B-0.00207-0.268640.516420.0593*H7C-0.00159-0.567600.532130.0593*H80.201660.414330.382650.0377*H5A-0.166230.998470.079090.0729*H5B0.04750-0.100200.275100.0479*H6A0.297090.189080.279880.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H2A	0.26884	-0.54591	0.53860	0.0649*
H3A-0.160590.324390.336560.0569*H3B-0.083720.201240.366680.0569*H50.40001-0.117470.474860.0464*H60.337400.195150.422240.0444*H7A0.01136-0.490860.476850.0593*H7B-0.00207-0.268640.516420.0593*H7C-0.00159-0.567600.532130.0593*H80.201660.414330.382650.0377*H5A-0.166230.998470.079090.0729*H5B0.04750-0.100200.275100.0479*H6A0.297090.189080.279880.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H2B	0.08747	0.62892	0.34795	0.0490*
H3B-0.083720.201240.366680.0569*H50.40001-0.117470.474860.0464*H60.337400.195150.422240.0444*H7A0.01136-0.490860.476850.0593*H7B-0.00207-0.268640.516420.0593*H7C-0.00159-0.567600.532130.0593*H80.201660.414330.382650.0377*H5A-0.166230.998470.079090.0729*H5B0.04750-0.100200.275100.0479*H6A0.297090.189080.279880.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H3A	-0.16059	0.32439	0.33656	0.0569*
H50.40001-0.117470.474860.0464*H60.337400.195150.422240.0444*H7A0.01136-0.490860.476850.0593*H7B-0.00207-0.268640.516420.0593*H7C-0.00159-0.567600.532130.0593*H80.201660.414330.382650.0377*H5A-0.166230.998470.079090.0729*H5B0.04750-0.100200.275100.0479*H6A0.297090.189080.279880.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H3B	-0.08372	0.20124	0.36668	0.0569*
H60.337400.195150.422240.0444*H7A0.01136-0.490860.476850.0593*H7B-0.00207-0.268640.516420.0593*H7C-0.00159-0.567600.532130.0593*H80.201660.414330.382650.0377*H5A-0.166230.998470.079090.0729*H5B0.04750-0.100200.275100.0479*H6A0.297090.189080.279880.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	Н5	0.40001	-0.11747	0.47486	0.0464*
H7A0.01136-0.490860.476850.0593*H7B-0.00207-0.268640.516420.0593*H7C-0.00159-0.567600.532130.0593*H80.201660.414330.382650.0377*H5A-0.166230.998470.079090.0729*H5B0.04750-0.100200.275100.0479*H6A0.297090.189080.279880.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H6	0.33740	0.19515	0.42224	0.0444*
H7B-0.00207-0.268640.516420.0593*H7C-0.00159-0.567600.532130.0593*H80.201660.414330.382650.0377*H5A-0.166230.998470.079090.0729*H5B0.04750-0.100200.275100.0479*H6A0.297090.189080.279880.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H7A	0.01136	-0.49086	0.47685	0.0593*
H7C-0.00159-0.567600.532130.0593*H80.201660.414330.382650.0377*H5A-0.166230.998470.079090.0729*H5B0.04750-0.100200.275100.0479*H6A0.297090.189080.279880.0534*H6B0.218350.319470.252170.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H7B	-0.00207	-0.26864	0.51642	0.0593*
H80.201660.414330.382650.0377*H5A-0.166230.998470.079090.0729*H5B0.04750-0.100200.275100.0479*H6A0.297090.189080.279880.0534*H6B0.218350.319470.252170.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H7C	-0.00159	-0.56760	0.53213	0.0593*
H5A-0.166230.998470.079090.0729*H5B0.04750-0.100200.275100.0479*H6A0.297090.189080.279880.0534*H6B0.218350.319470.252170.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H8	0.20166	0.41433	0.38265	0.0377*
H5B0.04750-0.100200.275100.0479*H6A0.297090.189080.279880.0534*H6B0.218350.319470.252170.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H5A	-0.16623	0.99847	0.07909	0.0729*
H6A0.297090.189080.279880.0534*H6B0.218350.319470.252170.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H5B	0.04750	-0.10020	0.27510	0.0479*
H6B0.218350.319470.252170.0534*H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H6A	0.29709	0.18908	0.27988	0.0534*
H110.045950.615460.173850.0351*H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H6B	0.21835	0.31947	0.25217	0.0534*
H14-0.278770.522690.140880.0458*H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H11	0.04595	0.61546	0.17385	0.0351*
H15-0.205770.252490.197300.0421*H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H14	-0.27877	0.52269	0.14088	0.0458*
H16A0.112460.819830.102660.0675*H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H15	-0.20577	0.25249	0.19730	0.0421*
H16B0.095611.037010.142840.0675*H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H16A	0.11246	0.81983	0.10266	0.0675*
H16C0.102261.118260.087490.0675*H17-0.068190.087110.239960.0368*	H16B	0.09561	1.03701	0.14284	0.0675*
H17 -0.06819 0.08711 0.23996 0.0368*	H16C	0.10226	1.11826	0.08749	0.0675*
	H17	-0.06819	0.08711	0.23996	0.0368*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
01	0.028 (3)	0.070 (4)	0.055 (4)	-0.003 (3)	-0.004 (3)	0.032 (3)
O2	0.030 (3)	0.052 (4)	0.049 (3)	0.005 (2)	-0.003 (2)	0.013 (3)
O3	0.028 (2)	0.039 (3)	0.060 (3)	0.000 (2)	-0.011 (2)	0.016 (3)
N1	0.031 (3)	0.031 (4)	0.042 (4)	0.001 (3)	-0.010 (3)	0.012 (3)
N2	0.024 (3)	0.036 (4)	0.062 (4)	-0.005(3)	-0.013 (3)	0.013 (3)
N3	0.026 (3)	0.055 (5)	0.062 (4)	-0.003(3)	-0.010 (3)	0.020 (4)
C1	0.025 (4)	0.038 (5)	0.030 (4)	0.000 (3)	0.001 (3)	0.005 (3)
C2	0.029 (4)	0.037 (5)	0.040 (4)	0.007 (4)	-0.007(3)	0.001 (4)
C3	0.029 (4)	0.039 (5)	0.026 (4)	0.000 (3)	0.003 (3)	0.003 (3)
C4	0.036 (4)	0.033 (4)	0.023 (4)	0.010 (4)	-0.005 (3)	-0.002 (3)
C5	0.024 (4)	0.039 (5)	0.054 (5)	0.001 (3)	-0.004 (3)	0.007 (4)
C6	0.029 (4)	0.033 (5)	0.049 (5)	-0.002(3)	0.003 (3)	0.007 (4)
C7	0.027 (4)	0.074 (6)	0.047 (5)	-0.009 (4)	-0.003 (4)	0.006 (4)
C8	0.033 (4)	0.032 (4)	0.030 (4)	-0.005 (4)	0.003 (3)	0.000 (3)
C9	0.023 (4)	0.032 (4)	0.038 (4)	0.001 (3)	0.002 (3)	-0.005 (4)
O4	0.026 (2)	0.045 (3)	0.053 (3)	0.002 (2)	0.004 (2)	0.018 (3)
05	0.036 (3)	0.056 (4)	0.054 (4)	0.008 (3)	-0.008(3)	0.023 (3)
O6	0.037 (3)	0.037 (3)	0.055 (3)	0.006 (2)	-0.013 (3)	0.016 (3)
N4	0.033 (3)	0.032 (3)	0.027 (3)	0.001 (3)	-0.003 (2)	0.008 (3)
N5	0.037 (3)	0.035 (4)	0.048 (4)	-0.008(3)	-0.009(3)	0.019 (3)
N6	0.028 (3)	0.041 (4)	0.064 (5)	-0.004(3)	-0.007(3)	0.011 (3)
C10	0.035 (4)	0.033 (4)	0.024 (4)	-0.001 (4)	-0.006 (3)	-0.004 (3)
C11	0.023 (3)	0.038 (4)	0.027 (4)	-0.001 (3)	-0.003 (3)	-0.001 (4)
C12	0.031 (4)	0.025 (4)	0.035 (4)	-0.002(3)	-0.001(3)	-0.002(3)
C13	0.029 (4)	0.040 (5)	0.027 (4)	0.006 (4)	-0.002(3)	0.005 (4)
C14	0.022 (3)	0.050 (5)	0.043 (5)	0.000 (4)	-0.005(3)	-0.001 (4)
C15	0.026 (3)	0.039 (4)	0.041 (4)	-0.006 (4)	0.001 (3)	0.012 (4)
C16	0.027 (4)	0.052 (5)	0.056 (6)	-0.008 (4)	0.000 (4)	0.005 (4)
C17	0.027 (4)	0.031 (4)	0.033 (4)	0.004 (3)	-0.007 (3)	0.004 (3)
C18	0.030 (4)	0.032 (4)	0.038 (4)	-0.004 (4)	-0.002(3)	-0.005 (4)

Atomic displacement parameters  $(Å^2)$ 

# Geometric parameters (Å, °)

01—C3	1.365 (8)	C1—C8	1.444 (9)
O1—C7	1.418 (7)	C2—C3	1.386 (9)
O2—C4	1.373 (8)	C3—C4	1.379 (9)
O3—C9	1.232 (8)	C4—C5	1.371 (9)
O2—H2A	0.8200	C5—C6	1.383 (8)
O4—C12	1.365 (8)	C2—H2	0.9300
O4—C16	1.426 (7)	C5—H5	0.9300
O5—C13	1.374 (8)	С6—Н6	0.9300
O6—C18	1.244 (8)	C7—H7C	0.9600
O5—H5A	0.8200	C7—H7A	0.9600
N1—C8	1.259 (9)	C7—H7B	0.9600
N1—N2	1.377 (8)	C8—H8	0.9300
N2—C9	1.375 (7)	C10—C11	1.409 (9)
N3—C9	1.335 (9)	C10—C15	1.384 (8)

N2—H2B	0.8600	C10—C17	1.456 (8)
N3—H3B	0.8600	C11—C12	1.388 (9)
N3—H3A	0.8600	C12—C13	1.404 (9)
N4—N5	1.375 (7)	C13—C14	1.373 (9)
N4—C17	1.282 (7)	C14—C15	1.372 (10)
N5—C18	1.353 (9)	C11—H11	0.9300
N6—C18	1.336 (9)	C14—H14	0.9300
N5—H5B	0.8600	С15—Н15	0.9300
N6—H6B	0.8600	C16—H16A	0.9600
N6—H6A	0.8600	C16—H16B	0.9600
C1—C2	1.386 (9)	C16—H16C	0.9600
C1—C6	1.390 (8)	С17—Н17	0.9300
C3—O1—C7	117.9 (5)	С5—С6—Н6	119.00
C4—O2—H2A	109.00	H7A—C7—H7C	109.00
C12—O4—C16	117.8 (5)	H7A—C7—H7B	109.00
C13—O5—H5A	109.00	O1—C7—H7B	109.00
N2—N1—C8	116.3 (5)	O1—C7—H7C	109.00
N1—N2—C9	121.6 (5)	O1—C7—H7A	109.00
C9—N2—H2B	119.00	H7B—C7—H7C	110.00
N1—N2—H2B	119.00	C1—C8—H8	119.00
C9—N3—H3A	120.00	N1—C8—H8	118.00
H3A—N3—H3B	120.00	C11—C10—C15	119.1 (5)
C9—N3—H3B	120.00	C15—C10—C17	119.2 (5)
N5—N4—C17	114.3 (5)	C11—C10—C17	121.6 (5)
N4—N5—C18	122.7 (5)	C10—C11—C12	119.4 (5)
C18—N5—H5B	119.00	C11—C12—C13	119.5 (6)
N4—N5—H5B	119.00	O4—C12—C11	126.7 (6)
H6A—N6—H6B	120.00	O4—C12—C13	113.7 (5)
C18—N6—H6A	120.00	O5—C13—C14	119.4 (5)
C18—N6—H6B	120.00	O5—C13—C12	119.6 (5)
C2—C1—C6	118.0 (6)	C12—C13—C14	121.0 (6)
C2—C1—C8	120.9 (6)	C13—C14—C15	119.0 (6)
C6—C1—C8	121.1 (6)	C10-C15-C14	121.9 (6)
C1—C2—C3	120.7 (6)	N4—C17—C10	122.8 (5)
O1—C3—C2	126.4 (5)	N5-C18-N6	115.7 (6)
C2—C3—C4	120.0 (6)	O6—C18—N5	120.4 (6)
O1—C3—C4	113.5 (5)	O6—C18—N6	123.8 (6)
O2—C4—C5	119.0 (6)	C10—C11—H11	120.00
O2—C4—C3	120.7 (6)	C12—C11—H11	120.00
C3—C4—C5	120.4 (6)	C13—C14—H14	120.00
C4—C5—C6	119.3 (5)	C15—C14—H14	120.00
C1—C6—C5	121.6 (6)	C10—C15—H15	119.00
N1—C8—C1	123.1 (6)	C14—C15—H15	119.00
O3—C9—N2	120.3 (6)	O4—C16—H16A	110.00
N2—C9—N3	115.6 (6)	O4—C16—H16B	109.00
O3—C9—N3	124.1 (5)	O4—C16—H16C	110.00
С3—С2—Н2	120.00	H16A—C16—H16B	109.00
C1—C2—H2	120.00	H16A—C16—H16C	109.00

С6—С5—Н5	120.00	H16B—C16—H16C	109.00
С4—С5—Н5	120.00	N4—C17—H17	119.00
С1—С6—Н6	119.00	С10—С17—Н17	119.00
C7—O1—C3—C2	6.5 (9)	O1—C3—C4—O2	3.3 (8)
C7—O1—C3—C4	-176.1 (6)	O1—C3—C4—C5	-177.0 (5)
C16-04-C12-C11	2.9 (9)	C2—C3—C4—C5	0.6 (9)
C16-04-C12-C13	-175.3 (6)	C3—C4—C5—C6	0.4 (9)
C8—N1—N2—C9	172.7 (6)	O2—C4—C5—C6	-180.0 (5)
N2-N1-C8-C1	176.9 (5)	C4—C5—C6—C1	-1.5 (9)
N1—N2—C9—N3	-2.0 (8)	C15-C10-C11-C12	-0.8 (9)
N1—N2—C9—O3	179.3 (6)	C17—C10—C11—C12	175.9 (6)
C17—N4—N5—C18	-175.8 (6)	C11—C10—C15—C14	0.5 (9)
N5—N4—C17—C10	-176.6 (5)	C17—C10—C15—C14	-176.2 (6)
N4—N5—C18—O6	-177.8 (5)	C11—C10—C17—N4	1.8 (9)
N4—N5—C18—N6	0.3 (9)	C15—C10—C17—N4	178.5 (6)
C6-C1-C8-N1	175.4 (6)	C10-C11-C12-O4	-178.3 (6)
C2-C1-C6-C5	1.5 (9)	C10-C11-C12-C13	-0.2 (9)
C6—C1—C2—C3	-0.4 (10)	O4—C12—C13—O5	0.2 (8)
C8—C1—C2—C3	-178.8 (6)	O4—C12—C13—C14	179.8 (6)
C8—C1—C6—C5	179.8 (6)	C11—C12—C13—O5	-178.2 (5)
C2-C1-C8-N1	-6.3 (10)	C11—C12—C13—C14	1.4 (9)
C1—C2—C3—C4	-0.6 (10)	O5—C13—C14—C15	178.0 (6)
C1—C2—C3—O1	176.7 (6)	C12—C13—C14—C15	-1.7 (10)
C2—C3—C4—O2	-179.0 (6)	C13—C14—C15—C10	0.7 (10)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
02—H2A…O1	0.82	2.17	2.627 (6)	115
O2— $H2A$ ···O5 <sup>i</sup>	0.82	2.34	3.108 (7)	156
N2—H2 <i>B</i> ···O6 <sup>ii</sup>	0.86	2.11	2.923 (7)	158
N3—H3A····O6 <sup>iii</sup>	0.86	2.16	2.987 (7)	162
N3—H3 <i>B</i> ···N1	0.86	2.31	2.674 (8)	106
O5—H5 <i>A</i> …O4	0.82	2.18	2.632 (6)	115
N5—H5 <i>B</i> ···O3 <sup>iv</sup>	0.86	2.08	2.909 (7)	161
N6—H6A····O3 <sup>v</sup>	0.86	2.13	2.965 (7)	164
N6—H6 <i>B</i> …N4	0.86	2.32	2.677 (7)	105

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