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(*E*)-Methyl *N*′-(3-methoxybenzylidene)-hydrazinecarboxylate

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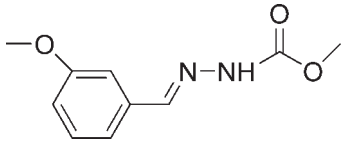
Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.109; data-to-parameter ratio = 13.7.

The title compound, $C_{10}H_{12}N_2O_3$, crystallizes with two independent molecules in the asymmetric unit which differ in the orientation of the methoxy group. Each independent molecule adopts a *trans* configuration with respect to the C=N bond. In the crystal structure, molecules are linked into chains running along [001] by N—H···O and N—H···N hydrogen bonds. In addition, an intermolecular C—H···π interaction is observed.

Related literature

For general background to the properties of benzaldehyde-hydrazone derivatives, see: Parashar *et al.* (1988); Hadjoudis *et al.* (1987); Borg *et al.* (1999); Kahwa *et al.* (1986); Santos *et al.* (2001). For a related structure, see: Shang *et al.* (2007).



Experimental

Crystal data

$C_{10}H_{12}N_2O_3$
M_r = 208.22
Monoclinic, $P2_1/c$
a = 18.207 (3) Å
b = 7.3677 (12) Å
c = 16.552 (3) Å
β = 104.243 (5)°
V = 2152.1 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 223 K
0.24 × 0.21 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.977, T_{max} = 0.989
11364 measured reflections
3790 independent reflections
3033 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.109
S = 1.07
3790 reflections
276 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O5	0.86	2.07	2.9188 (18)	172
N4—H4···O2^{i}	0.86	2.25	2.8365 (17)	126
N4—H4···N1^{i}	0.86	2.55	3.3883 (19)	164
C11—H11B···$Cg1^{ii}$	0.96	2.91	3.776 (3)	150

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x+1, -y+1, -z+1$. $Cg1$ is the centroid of the C12–C17 ring.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2891).

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(*E*)-Methyl *N*′-(3-methoxybenzylidene)hydrazinecarboxylate

Lu-Ping Lv, Wen-Bo Yu, Chun-Yu Huang, Wei-Wei Li and Xian-Chao Hu

S1. Comment

Benzaldehydehydrazone derivatives have attracted much attention due to their pharmacological activity (Parashar *et al.*, 1988) and their photochromic properties (Hadjoudis *et al.*, 1987). They are important intermediates of 1,3,4-oxadiazoles, which have been reported to be versatile compounds with many interesting properties (Borg *et al.*, 1999). Metal complexes based on Schiff bases have received considerable attention because they can be utilized as model compounds of active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). We report here the crystal structure of the title compound (Fig. 1).

The title compound contains two independent, but almost identical molecules in the asymmetric unit. Each independent molecule adopts a *trans* configuration with respect to the C═N bond. The N1/N2/O2/O3/C8/C9/C10 and N3/N4/O5/O6/C18/C19/C20 planes form dihedral angles of 4.51 (6)° and 13.80 (6)°, respectively, with the C2—C7 and C12—C17 planes. The dihedral angle between the two independent benzene rings is 59.18 (6)°. Bond lengths and angles are comparable to those observed for methyl*N*′-[(*E*)-4-methoxybenzylidene]hydrazinecarboxylate (Shang *et al.*, 2007).

In the crystal structure, molecules are linked into chains running along the [001] by N—H···O and N—H···N hydrogen bonds. In addition, an intermolecular C—H···π interaction is observed (Table 1).

S2. Experimental

3-Methoxybenzaldehyde (1.36 g, 0.01 mol) and methyl hydrazinecarboxylate (0.90 g, 0.01 mol) were dissolved in stirred methanol (20 ml) and left for 2.5 h at room temperature. The resulting solid was filtered off and recrystallized from ethanol to give the title compound in 95% yield. Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature (m.p. 436–438 K).

S3. Refinement

H atoms were positioned geometrically (N-H = 0.86 Å and C-H = 0.93 or 0.96 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C,N) and 1.5U_{eq}(C_{methyl}). A rotating group model was used for the methyl groups.

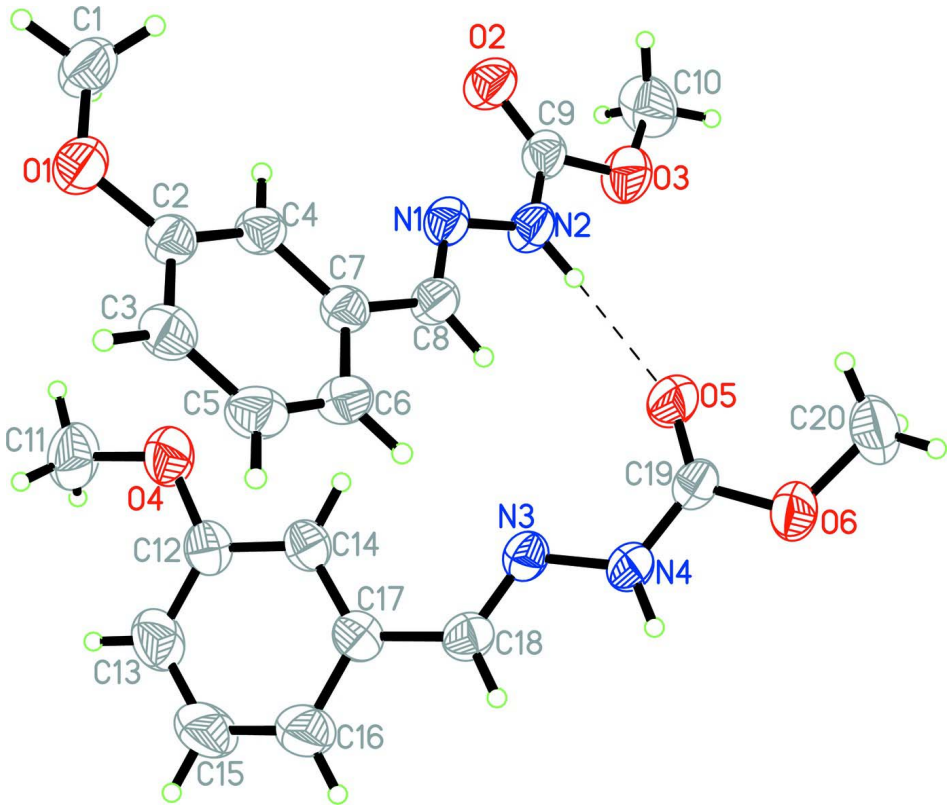

Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 40% probability level. The dashed line indicates a hydrogen bond.

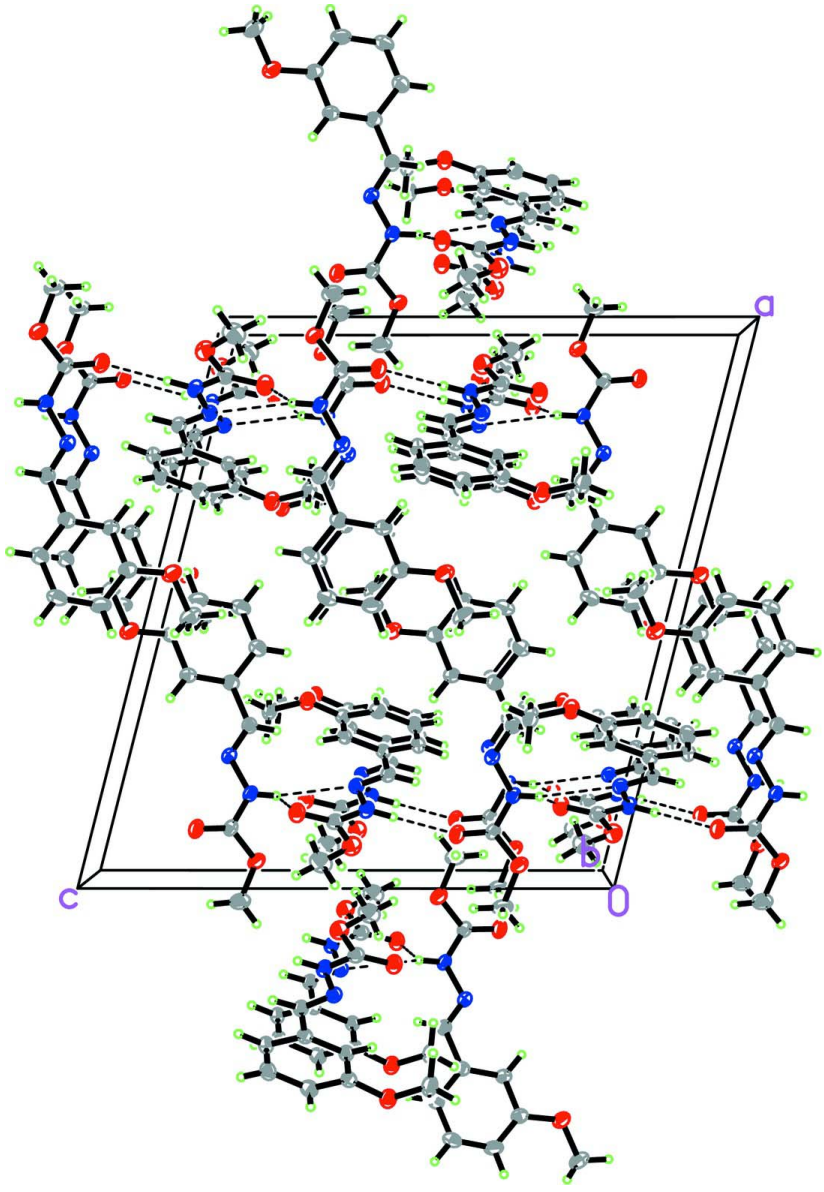

Figure 2

Crystal packing of the title compound. Hydrogen bonds are shown as dashed lines.

(*E*)-Methyl *N*′-(3-methoxybenzylidene)hydrazinecarboxylate

Crystal data

$C_{10}H_{12}N_2O_3$
$M_r = 208.22$
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$a = 18.207\ (3)$ Å
$b = 7.3677\ (12)$ Å
$c = 16.552\ (3)$ Å
$\beta = 104.243\ (5)°$
$V = 2152.1\ (6)$ Å^3
$Z = 8$

$F(000) = 880$
$D_x = 1.285$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3790 reflections
$\theta = 2.3–25.0°$
$\mu = 0.10$ mm^{-1}
$T = 223$ K
Block, colourless
0.24 × 0.21 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.977, T_{max} = 0.989
11364 measured reflections
3790 independent reflections
3033 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −21→18
k = −8→8
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.109
S = 1.07
3790 reflections
276 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 0.3311P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0115 (12)

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. 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 $F^2 > 2$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	*y*	*z*	U_{iso}*/U_{eq}
O1	0.68188 (7)	1.33813 (15)	−0.17091 (7)	0.0626 (3)
O2	0.86739 (7)	0.49630 (16)	−0.12622 (7)	0.0661 (3)
O3	0.92117 (7)	0.34574 (16)	−0.00794 (8)	0.0717 (4)
O4	0.55036 (7)	0.73143 (19)	−0.03581 (8)	0.0788 (4)
O5	0.90715 (7)	0.5763 (2)	0.18325 (7)	0.0792 (4)
O6	0.96333 (6)	0.64573 (18)	0.31586 (7)	0.0690 (4)
N1	0.82614 (7)	0.75999 (16)	−0.02931 (7)	0.0491 (3)
N2	0.86458 (7)	0.60387 (17)	0.00177 (8)	0.0545 (3)
H2	0.8769	0.5836	0.0546	0.065*
N3	0.77335 (7)	0.69523 (16)	0.21361 (7)	0.0492 (3)
N4	0.84157 (7)	0.68885 (19)	0.27209 (8)	0.0574 (4)
H4	0.8442	0.7210	0.3227	0.069*
C1	0.69744 (12)	1.2445 (3)	−0.23962 (10)	0.0724 (5)
H1A	0.6782	1.3132	−0.2896	0.109*
H1B	0.6735	1.1276	−0.2449	0.109*

H1C	0.7512	1.2294	−0.2309	0.109*
C2	0.70930 (8)	1.2656 (2)	−0.09344 (9)	0.0482 (4)
C3	0.70053 (9)	1.3743 (2)	−0.02757 (10)	0.0559 (4)
H3	0.6774	1.4873	−0.0382	0.067*
C4	0.74387 (8)	1.0972 (2)	−0.07774 (9)	0.0478 (4)
H4A	0.7500	1.0249	−0.1217	0.057*
C5	0.72602 (10)	1.3148 (2)	0.05299 (10)	0.0612 (4)
H5	0.7204	1.3879	0.0969	0.073*
C6	0.76013 (9)	1.1460 (2)	0.06930 (10)	0.0567 (4)
H6	0.7768	1.1058	0.1240	0.068*
C7	0.76944 (8)	1.0368 (2)	0.00429 (9)	0.0475 (4)
C8	0.80804 (9)	0.8620 (2)	0.02498 (9)	0.0510 (4)
H8	0.8199	0.8239	0.0802	0.061*
C9	0.88263 (9)	0.4835 (2)	−0.05143 (10)	0.0522 (4)
C10	0.94571 (13)	0.2072 (3)	−0.05631 (15)	0.0888 (6)
H10A	0.9814	0.1291	−0.0201	0.133*
H10B	0.9694	0.2625	−0.0960	0.133*
H10C	0.9028	0.1373	−0.0853	0.133*
C11	0.47641 (11)	0.7249 (3)	−0.09038 (13)	0.0860 (6)
H11A	0.4804	0.7021	−0.1463	0.129*
H11B	0.4513	0.8388	−0.0885	0.129*
H11C	0.4478	0.6293	−0.0731	0.129*
C12	0.55619 (9)	0.7559 (2)	0.04734 (10)	0.0567 (4)
C13	0.49554 (11)	0.7833 (3)	0.08170 (14)	0.0777 (6)
H13	0.4464	0.7862	0.0480	0.093*
C14	0.62919 (9)	0.7513 (2)	0.09829 (10)	0.0518 (4)
H14	0.6700	0.7337	0.0747	0.062*
C15	0.50852 (12)	0.8064 (4)	0.16661 (15)	0.0962 (7)
H15	0.4676	0.8253	0.1899	0.115*
C16	0.58066 (11)	0.8024 (3)	0.21795 (13)	0.0812 (6)
H16	0.5882	0.8194	0.2751	0.097*
C17	0.64204 (9)	0.7725 (2)	0.18355 (10)	0.0531 (4)
C18	0.71842 (9)	0.7617 (2)	0.23885 (10)	0.0528 (4)
H18	0.7269	0.8041	0.2933	0.063*
C19	0.90395 (9)	0.6325 (2)	0.25016 (9)	0.0504 (4)
C20	1.03667 (10)	0.6043 (3)	0.30340 (14)	0.0839 (6)
H20A	1.0750	0.6610	0.3463	0.126*
H20B	1.0401	0.6489	0.2500	0.126*
H20C	1.0441	0.4752	0.3056	0.126*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0750 (8)	0.0619 (7)	0.0499 (6)	0.0148 (6)	0.0135 (5)	0.0052 (5)
O2	0.0832 (8)	0.0608 (7)	0.0546 (7)	0.0141 (6)	0.0177 (6)	0.0080 (5)
O3	0.0808 (9)	0.0605 (7)	0.0716 (8)	0.0215 (6)	0.0150 (6)	0.0188 (6)
O4	0.0582 (8)	0.1052 (10)	0.0640 (8)	0.0062 (7)	−0.0020 (6)	−0.0096 (7)
O5	0.0762 (9)	0.1133 (11)	0.0448 (7)	0.0302 (8)	0.0089 (6)	−0.0079 (7)

O6	0.0538 (7)	0.0895 (9)	0.0555 (7)	0.0082 (6)	−0.0021 (5)	−0.0090 (6)
N1	0.0505 (8)	0.0482 (7)	0.0468 (7)	0.0021 (6)	0.0085 (6)	0.0069 (5)
N2	0.0622 (8)	0.0538 (7)	0.0444 (7)	0.0074 (6)	0.0071 (6)	0.0094 (6)
N3	0.0509 (8)	0.0497 (7)	0.0434 (7)	−0.0003 (6)	0.0045 (6)	−0.0027 (5)
N4	0.0532 (8)	0.0758 (9)	0.0387 (7)	0.0044 (7)	0.0026 (6)	−0.0129 (6)
C1	0.0914 (14)	0.0770 (12)	0.0465 (9)	0.0169 (10)	0.0127 (9)	0.0039 (8)
C2	0.0458 (9)	0.0518 (8)	0.0477 (8)	−0.0018 (7)	0.0126 (6)	0.0009 (6)
C3	0.0568 (10)	0.0507 (8)	0.0629 (10)	0.0035 (7)	0.0201 (8)	−0.0039 (7)
C4	0.0493 (9)	0.0511 (8)	0.0437 (8)	−0.0004 (7)	0.0129 (6)	−0.0042 (6)
C5	0.0685 (11)	0.0645 (10)	0.0544 (10)	0.0014 (9)	0.0226 (8)	−0.0122 (8)
C6	0.0589 (10)	0.0689 (10)	0.0438 (8)	−0.0003 (8)	0.0157 (7)	−0.0013 (7)
C7	0.0432 (8)	0.0536 (8)	0.0468 (8)	−0.0038 (7)	0.0132 (6)	0.0006 (6)
C8	0.0519 (9)	0.0573 (9)	0.0431 (8)	−0.0014 (7)	0.0104 (7)	0.0057 (7)
C9	0.0507 (9)	0.0493 (8)	0.0546 (9)	0.0015 (7)	0.0091 (7)	0.0112 (7)
C10	0.0927 (15)	0.0646 (11)	0.1145 (17)	0.0286 (11)	0.0360 (13)	0.0127 (11)
C11	0.0681 (13)	0.0987 (15)	0.0760 (13)	−0.0005 (11)	−0.0113 (10)	−0.0085 (11)
C12	0.0513 (10)	0.0520 (9)	0.0634 (11)	−0.0023 (7)	0.0077 (8)	−0.0035 (7)
C13	0.0454 (10)	0.0951 (14)	0.0882 (15)	−0.0051 (10)	0.0079 (9)	−0.0067 (11)
C14	0.0457 (9)	0.0492 (8)	0.0596 (9)	−0.0009 (7)	0.0112 (7)	−0.0031 (7)
C15	0.0515 (12)	0.152 (2)	0.0911 (16)	−0.0039 (13)	0.0284 (11)	−0.0137 (15)
C16	0.0600 (12)	0.1185 (17)	0.0685 (12)	−0.0066 (11)	0.0224 (10)	−0.0107 (11)
C17	0.0496 (9)	0.0503 (8)	0.0601 (10)	−0.0052 (7)	0.0149 (7)	−0.0030 (7)
C18	0.0571 (10)	0.0539 (9)	0.0467 (8)	−0.0048 (7)	0.0116 (7)	−0.0053 (7)
C19	0.0565 (10)	0.0491 (8)	0.0414 (8)	0.0052 (7)	0.0044 (7)	0.0021 (6)
C20	0.0541 (12)	0.0970 (15)	0.0941 (15)	0.0160 (10)	0.0058 (10)	0.0073 (12)

Geometric parameters (Å, º)

O1—C2	1.3654 (18)	C5—C6	1.387 (2)
O1—C1	1.417 (2)	C5—H5	0.93
O2—C9	1.2039 (18)	C6—C7	1.387 (2)
O3—C9	1.3387 (18)	C6—H6	0.93
O3—C10	1.435 (2)	C7—C8	1.467 (2)
O4—C12	1.366 (2)	C8—H8	0.93
O4—C11	1.426 (2)	C10—H10A	0.96
O5—C19	1.1971 (18)	C10—H10B	0.96
O6—C19	1.3351 (18)	C10—H10C	0.96
O6—C20	1.433 (2)	C11—H11A	0.96
N1—C8	1.2757 (19)	C11—H11B	0.96
N1—N2	1.3785 (17)	C11—H11C	0.96
N2—C9	1.346 (2)	C12—C13	1.376 (3)
N2—H2	0.86	C12—C14	1.388 (2)
N3—C18	1.273 (2)	C13—C15	1.377 (3)
N3—N4	1.3749 (17)	C13—H13	0.93
N4—C19	1.341 (2)	C14—C17	1.381 (2)
N4—H4	0.86	C14—H14	0.93
C1—H1A	0.96	C15—C16	1.378 (3)
C1—H1B	0.96	C15—H15	0.93

C1—H1C	0.96	C16—C17	1.391 (2)
C2—C4	1.386 (2)	C16—H16	0.93
C2—C3	1.393 (2)	C17—C18	1.467 (2)
C3—C5	1.372 (2)	C18—H18	0.93
C3—H3	0.93	C20—H20A	0.96
C4—C7	1.396 (2)	C20—H20B	0.96
C4—H4A	0.93	C20—H20C	0.96

C2—O1—C1	117.64 (12)	O3—C10—H10A	109.5
C9—O3—C10	115.68 (14)	O3—C10—H10B	109.5
C12—O4—C11	118.03 (15)	H10A—C10—H10B	109.5
C19—O6—C20	117.62 (14)	O3—C10—H10C	109.5
C8—N1—N2	115.11 (12)	H10A—C10—H10C	109.5
C9—N2—N1	119.26 (12)	H10B—C10—H10C	109.5
C9—N2—H2	120.4	O4—C11—H11A	109.5
N1—N2—H2	120.4	O4—C11—H11B	109.5
C18—N3—N4	115.39 (13)	H11A—C11—H11B	109.5
C19—N4—N3	119.91 (12)	O4—C11—H11C	109.5
C19—N4—H4	120.0	H11A—C11—H11C	109.5
N3—N4—H4	120.0	H11B—C11—H11C	109.5
O1—C1—H1A	109.5	O4—C12—C13	124.38 (16)
O1—C1—H1B	109.5	O4—C12—C14	115.73 (15)
H1A—C1—H1B	109.5	C13—C12—C14	119.90 (16)
O1—C1—H1C	109.5	C12—C13—C15	119.10 (17)
H1A—C1—H1C	109.5	C12—C13—H13	120.4
H1B—C1—H1C	109.5	C15—C13—H13	120.4
O1—C2—C4	124.80 (13)	C17—C14—C12	120.93 (16)
O1—C2—C3	115.07 (13)	C17—C14—H14	119.5
C4—C2—C3	120.13 (14)	C12—C14—H14	119.5
C5—C3—C2	120.02 (15)	C13—C15—C16	121.65 (19)
C5—C3—H3	120.0	C13—C15—H15	119.2
C2—C3—H3	120.0	C16—C15—H15	119.2
C2—C4—C7	119.68 (14)	C15—C16—C17	119.41 (19)
C2—C4—H4A	120.2	C15—C16—H16	120.3
C7—C4—H4A	120.2	C17—C16—H16	120.3
C3—C5—C6	120.27 (15)	C14—C17—C16	119.00 (16)
C3—C5—H5	119.9	C14—C17—C18	121.84 (15)
C6—C5—H5	119.9	C16—C17—C18	119.15 (16)
C7—C6—C5	120.23 (15)	N3—C18—C17	121.13 (14)
C7—C6—H6	119.9	N3—C18—H18	119.4
C5—C6—H6	119.9	C17—C18—H18	119.4
C6—C7—C4	119.66 (14)	O5—C19—O6	124.39 (15)
C6—C7—C8	118.10 (13)	O5—C19—N4	126.52 (14)
C4—C7—C8	122.22 (14)	O6—C19—N4	109.08 (13)
N1—C8—C7	123.03 (13)	O6—C20—H20A	109.5
N1—C8—H8	118.5	O6—C20—H20B	109.5
C7—C8—H8	118.5	H20A—C20—H20B	109.5
O2—C9—O3	124.75 (15)	O6—C20—H20C	109.5

O2—C9—N2	126.11 (14)	H20A—C20—H20C	109.5
O3—C9—N2	109.14 (13)	H20B—C20—H20C	109.5
C8—N1—N2—C9	176.68 (14)	N1—N2—C9—O3	178.40 (12)
C18—N3—N4—C19	−175.58 (14)	C11—O4—C12—C13	−3.2 (3)
C1—O1—C2—C4	−7.6 (2)	C11—O4—C12—C14	176.59 (15)
C1—O1—C2—C3	172.35 (15)	O4—C12—C13—C15	180.0 (2)
O1—C2—C3—C5	179.99 (15)	C14—C12—C13—C15	0.2 (3)
C4—C2—C3—C5	−0.1 (2)	O4—C12—C14—C17	−179.29 (14)
O1—C2—C4—C7	−179.72 (14)	C13—C12—C14—C17	0.5 (2)
C3—C2—C4—C7	0.4 (2)	C12—C13—C15—C16	−0.2 (4)
C2—C3—C5—C6	−0.4 (3)	C13—C15—C16—C17	−0.6 (4)
C3—C5—C6—C7	0.7 (3)	C12—C14—C17—C16	−1.3 (2)
C5—C6—C7—C4	−0.4 (2)	C12—C14—C17—C18	177.79 (14)
C5—C6—C7—C8	178.06 (15)	C15—C16—C17—C14	1.3 (3)
C2—C4—C7—C6	−0.1 (2)	C15—C16—C17—C18	−177.8 (2)
C2—C4—C7—C8	−178.51 (13)	N4—N3—C18—C17	−178.49 (13)
N2—N1—C8—C7	177.72 (13)	C14—C17—C18—N3	−15.0 (2)
C6—C7—C8—N1	−172.84 (15)	C16—C17—C18—N3	164.04 (17)
C4—C7—C8—N1	5.6 (2)	C20—O6—C19—O5	5.5 (2)
C10—O3—C9—O2	0.7 (2)	C20—O6—C19—N4	−175.48 (15)
C10—O3—C9—N2	−178.90 (15)	N3—N4—C19—O5	−3.8 (3)
N1—N2—C9—O2	−1.2 (2)	N3—N4—C19—O6	177.20 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O5	0.86	2.07	2.9188 (18)	172
N4—H4···O2^{i}	0.86	2.25	2.8365 (17)	126
N4—H4···N1^{i}	0.86	2.55	3.3883 (19)	164
C11—H11*B*···*Cg*1^{ii}	0.96	2.91	3.776 (3)	150

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1.