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# Methyl *N*′-[(*E*)-2-methoxybenzylidene]-hydrazinecarboxylate

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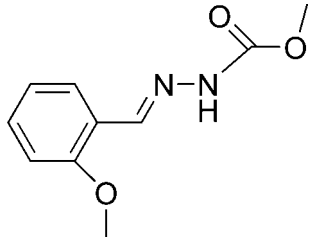
Key indicators: single-crystal X-ray study; $T$ = 223 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.041; $wR$ factor = 0.120; data-to-parameter ratio = 13.7.

The title compound, $C_{10}H_{12}N_2O_3$, crystallizes with two independent molecules in the asymmetric unit. The side chains in the two independent molecules have slightly different orientations, with the C=N—N—C torsion angle being 169.19 (14)° in one of the molecules and −179.86 (14)° in the other. 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, N—H···N and C—H···O hydrogen bonds. In addition, an intermolecular C—H···$\pi$ interaction is observed.

## Related literature

For applications of benzaldehydehydrazone derviatives, see: Parashar *et al.* (1988); Hadjoudis *et al.* (1987); Borg *et al.* (1999). For metal complexes of Schiff base ligands, see: 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, $P2_1/c$
$a$ = 17.221 (5) Å
$b$ = 7.442 (2) Å
$c$ = 16.611 (6) Å
$\beta$ = 95.423 (12)°
$V$ = 2119.4 (12) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 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
11064 measured reflections
3723 independent reflections
2834 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
$S$ = 1.08
3723 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

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

*Cg*1 is the centroid of the C12–C17 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2N···O5 | 0.86 | 2.08 | 2.938 (2) | 173 |
| N4—H4N···N1$^{i}$ | 0.86 | 2.42 | 3.279 (2) | 177 |
| C1—H1*A*···O2$^{i}$ | 0.96 | 2.52 | 3.472 (2) | 170 |
| C11—H11*B*···*Cg*1$^{ii}$ | 0.96 | 2.87 | 3.826 (3) | 175 |

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

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: CI2777).

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# supporting information

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## Methyl *N*′-[(*E*)-2-methoxybenzylidene]hydrazinecarboxylate

**Lu-Ping Lv, Wen-Bo Yu, Zhong-Hao Lu, 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 and N3/N4/O5/O6/C18/C19 planes form dihedral angles of 3.20 (6)° and 11.61 (5)°, respectively, with the C2—C7 and C12—C17 planes. The dihedral angle between the two independent benzene rings is 49.19 (7)°. The bond lengths and angles are comparable to those observed for methyl*N*′-[(*E*)-4-methoxybenzylidene]hydrazinecarboxylate (Shang *et al.*, 2007).

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

### S2. Experimental

2-Methoxybenzaldehyde (1.36 g, 0.01 mol) and methyl hydrazinecarboxylate (0.90 g, 0.01 mol) were dissolved in stirred methanol (25 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. 428–430 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) = 1.2$U_{eq}$(C,N) and 1.5$U_{eq}$($C_{methyl}$). In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

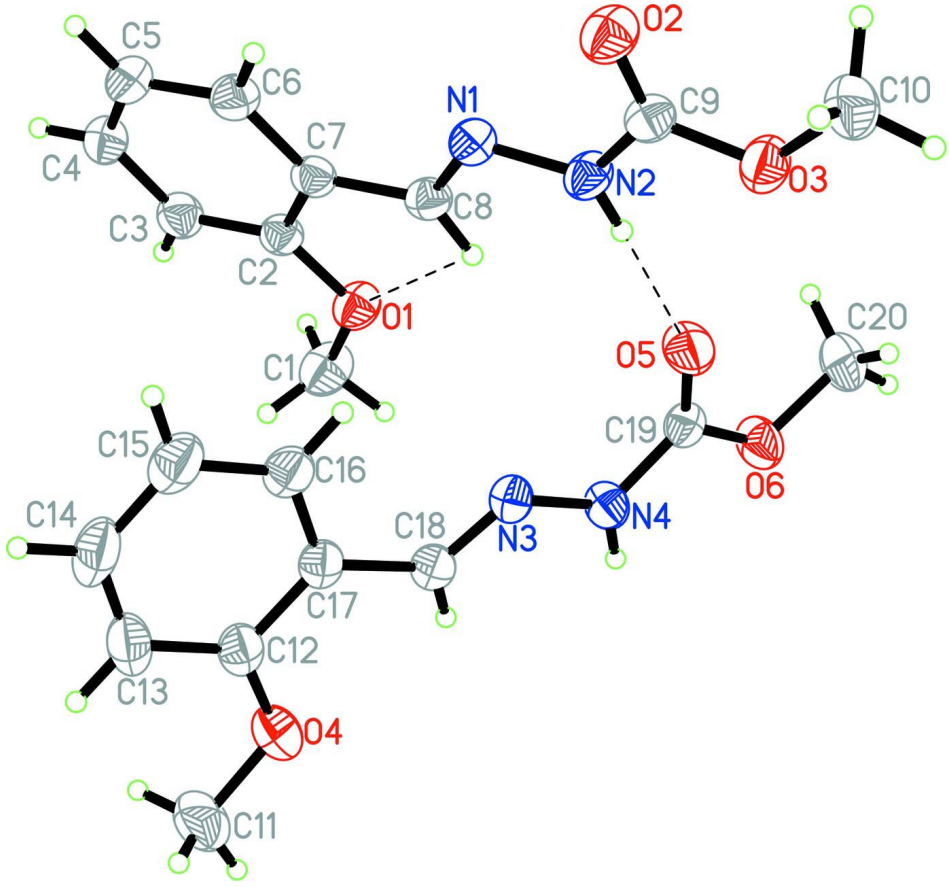


**Figure 1**

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines indicate hydrogen bonds.

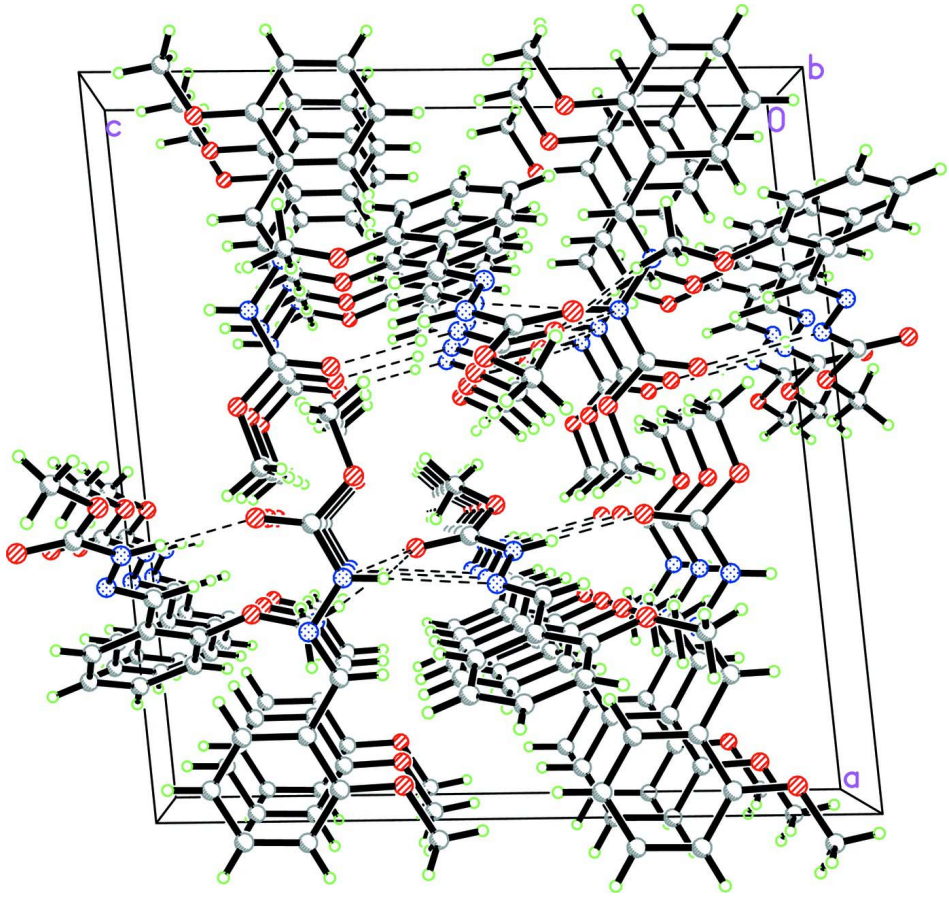


**Figure 2**

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

### Methyl *N*′-[(*E*)-2-methoxybenzylidene]hydrazinecarboxylate

*Crystal data*

$C_{10}H_{12}N_2O_3$
$M_r = 208.22$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 17.221\ (5)$ Å
$b = 7.442\ (2)$ Å
$c = 16.611\ (6)$ Å
$\beta = 95.423\ (12)°$
$V = 2119.4\ (12)$ Å$^3$
$Z = 8$
$F(000) = 880$
$D_x = 1.305$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3723 reflections
$\theta = 1.2–25.0°$
$\mu = 0.10$ 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
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.977$, $T_{max} = 0.989$
11064 measured reflections
3723 independent reflections
2834 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.2°$
$h = -20\rightarrow20$
$k = -8\rightarrow8$
$l = -19\rightarrow18$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.120$
$S = 1.08$
3723 reflections
271 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
$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2 + 0.1492P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å$^{-3}$
$\Delta\rho_{min} = -0.18$ e Å$^{-3}$

*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 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.27964 (7) | −0.12236 (16) | 0.66716 (7) | 0.0579 (3) |
| O3 | 0.41712 (7) | 0.63135 (17) | 0.50573 (7) | 0.0644 (4) |
| O2 | 0.36311 (7) | 0.49059 (17) | 0.39394 (7) | 0.0649 (4) |
| O6 | 0.45355 (6) | 0.3646 (2) | 0.82317 (7) | 0.0676 (4) |
| O4 | 0.06692 (7) | 0.15183 (19) | 0.84498 (9) | 0.0716 (4) |
| N3 | 0.26187 (7) | 0.29235 (18) | 0.74487 (8) | 0.0478 (3) |
| O5 | 0.40316 (7) | 0.3884 (2) | 0.69432 (8) | 0.0733 (4) |
| N1 | 0.31881 (7) | 0.21928 (19) | 0.49137 (8) | 0.0483 (3) |
| N2 | 0.35854 (8) | 0.37207 (19) | 0.51936 (8) | 0.0522 (4) |
| H2N | 0.3707 | 0.3869 | 0.5703 | 0.063* |
| N4 | 0.32825 (7) | 0.3208 (2) | 0.79597 (8) | 0.0525 (4) |
| H4N | 0.3270 | 0.3140 | 0.8475 | 0.063* |
| C7 | 0.26100 (8) | −0.0607 (2) | 0.52867 (9) | 0.0460 (4) |
| C17 | 0.13105 (9) | 0.1853 (2) | 0.72717 (11) | 0.0506 (4) |
| C18 | 0.20343 (9) | 0.2284 (2) | 0.77764 (10) | 0.0497 (4) |
| H18 | 0.2067 | 0.2093 | 0.8332 | 0.060* |
| C8 | 0.30274 (8) | 0.1085 (2) | 0.54641 (10) | 0.0479 (4) |
| H8 | 0.3183 | 0.1366 | 0.6001 | 0.057* |
| C9 | 0.37808 (9) | 0.4974 (2) | 0.46625 (10) | 0.0492 (4) |
| C16 | 0.12959 (10) | 0.1783 (3) | 0.64363 (12) | 0.0616 (5) |
| H16 | 0.1746 | 0.2063 | 0.6194 | 0.074* |
| C4 | 0.18349 (10) | −0.3883 (3) | 0.50054 (12) | 0.0635 (5) |
| H4 | 0.1581 | −0.4976 | 0.4910 | 0.076* |
| C3 | 0.21174 (10) | −0.3421 (2) | 0.57816 (11) | 0.0569 (5) |
| H3 | 0.2052 | −0.4199 | 0.6208 | 0.068* |

| | | | | |
|---|---|---|---|---|
| C5 | 0.19269 (10) | −0.2740 (3) | 0.43723 (11) | 0.0630 (5) |
| H5 | 0.1730 | −0.3054 | 0.3851 | 0.076* |
| C1 | 0.26395 (13) | −0.2246 (3) | 0.73518 (11) | 0.0735 (6) |
| H1A | 0.2882 | −0.1691 | 0.7833 | 0.110* |
| H1B | 0.2843 | −0.3438 | 0.7304 | 0.110* |
| H1C | 0.2086 | −0.2306 | 0.7382 | 0.110* |
| C2 | 0.25007 (8) | −0.1791 (2) | 0.59263 (10) | 0.0470 (4) |
| C20 | 0.53167 (10) | 0.3890 (3) | 0.80043 (15) | 0.0834 (7) |
| H20A | 0.5678 | 0.3901 | 0.8481 | 0.125* |
| H20B | 0.5348 | 0.5010 | 0.7722 | 0.125* |
| H20C | 0.5444 | 0.2922 | 0.7658 | 0.125* |
| C10 | 0.44366 (12) | 0.7734 (3) | 0.45624 (14) | 0.0771 (6) |
| H10A | 0.4707 | 0.8621 | 0.4901 | 0.116* |
| H10B | 0.3997 | 0.8279 | 0.4258 | 0.116* |
| H10C | 0.4783 | 0.7247 | 0.4198 | 0.116* |
| C6 | 0.23130 (10) | −0.1116 (3) | 0.45094 (11) | 0.0578 (5) |
| H6 | 0.2375 | −0.0354 | 0.4076 | 0.069* |
| C14 | −0.00378 (13) | 0.0922 (3) | 0.63078 (16) | 0.0853 (7) |
| H14 | −0.0489 | 0.0620 | 0.5984 | 0.102* |
| C19 | 0.39555 (9) | 0.3595 (2) | 0.76374 (10) | 0.0477 (4) |
| C13 | −0.00495 (11) | 0.0976 (3) | 0.71332 (16) | 0.0752 (6) |
| H13 | −0.0507 | 0.0708 | 0.7365 | 0.090* |
| C12 | 0.06241 (9) | 0.1433 (2) | 0.76246 (12) | 0.0582 (5) |
| C15 | 0.06312 (12) | 0.1308 (3) | 0.59552 (14) | 0.0783 (6) |
| H15 | 0.0636 | 0.1250 | 0.5396 | 0.094* |
| C11 | −0.00264 (13) | 0.1165 (3) | 0.88362 (16) | 0.0942 (8) |
| H11A | 0.0085 | 0.1268 | 0.9412 | 0.141* |
| H11B | −0.0208 | −0.0028 | 0.8703 | 0.141* |
| H11C | −0.0422 | 0.2019 | 0.8652 | 0.141* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0726 (7) | 0.0557 (8) | 0.0444 (7) | −0.0051 (6) | 0.0008 (5) | 0.0033 (5) |
| O3 | 0.0752 (8) | 0.0550 (8) | 0.0625 (8) | −0.0139 (6) | 0.0050 (6) | −0.0052 (6) |
| O2 | 0.0852 (8) | 0.0594 (9) | 0.0491 (8) | −0.0064 (6) | 0.0008 (6) | 0.0032 (6) |
| O6 | 0.0470 (6) | 0.0963 (11) | 0.0579 (8) | −0.0085 (6) | −0.0042 (5) | 0.0026 (7) |
| O4 | 0.0582 (7) | 0.0764 (10) | 0.0818 (10) | −0.0074 (6) | 0.0150 (6) | 0.0087 (7) |
| N3 | 0.0471 (7) | 0.0452 (8) | 0.0496 (8) | 0.0012 (6) | −0.0030 (6) | 0.0025 (6) |
| O5 | 0.0682 (8) | 0.1061 (12) | 0.0457 (8) | −0.0207 (7) | 0.0058 (6) | 0.0028 (7) |
| N1 | 0.0514 (7) | 0.0468 (9) | 0.0464 (8) | 0.0006 (6) | 0.0027 (6) | −0.0005 (7) |
| N2 | 0.0624 (8) | 0.0539 (10) | 0.0392 (7) | −0.0041 (7) | −0.0002 (6) | −0.0016 (6) |
| N4 | 0.0462 (7) | 0.0693 (10) | 0.0408 (7) | −0.0045 (6) | −0.0018 (6) | 0.0058 (7) |
| C7 | 0.0417 (8) | 0.0506 (10) | 0.0461 (9) | 0.0046 (7) | 0.0065 (6) | −0.0014 (8) |
| C17 | 0.0474 (8) | 0.0382 (10) | 0.0648 (11) | 0.0069 (7) | −0.0018 (7) | −0.0028 (8) |
| C18 | 0.0489 (9) | 0.0466 (10) | 0.0528 (10) | 0.0038 (7) | 0.0009 (7) | 0.0009 (8) |
| C8 | 0.0482 (8) | 0.0540 (11) | 0.0416 (9) | 0.0036 (7) | 0.0047 (7) | −0.0010 (8) |
| C9 | 0.0526 (9) | 0.0483 (11) | 0.0462 (10) | 0.0050 (7) | 0.0021 (7) | −0.0018 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C16 | 0.0562 (10) | 0.0587 (12) | 0.0681 (12) | 0.0111 (8) | −0.0036 (8) | −0.0107 (9) |
| C4 | 0.0579 (10) | 0.0629 (13) | 0.0704 (13) | −0.0092 (9) | 0.0093 (9) | −0.0139 (10) |
| C3 | 0.0579 (10) | 0.0535 (12) | 0.0605 (11) | −0.0032 (8) | 0.0110 (8) | 0.0008 (9) |
| C5 | 0.0601 (10) | 0.0758 (14) | 0.0525 (11) | −0.0061 (9) | 0.0012 (8) | −0.0149 (10) |
| C1 | 0.1031 (15) | 0.0659 (14) | 0.0504 (11) | −0.0079 (11) | 0.0014 (10) | 0.0094 (10) |
| C2 | 0.0439 (8) | 0.0485 (10) | 0.0488 (10) | 0.0050 (7) | 0.0058 (7) | −0.0025 (8) |
| C20 | 0.0483 (10) | 0.0993 (18) | 0.1017 (17) | −0.0118 (10) | 0.0030 (10) | −0.0090 (14) |
| C10 | 0.0798 (13) | 0.0608 (14) | 0.0931 (16) | −0.0161 (10) | 0.0202 (12) | −0.0003 (11) |
| C6 | 0.0569 (10) | 0.0692 (13) | 0.0477 (10) | −0.0006 (9) | 0.0067 (8) | −0.0018 (9) |
| C14 | 0.0684 (13) | 0.0708 (15) | 0.1093 (19) | 0.0035 (11) | −0.0308 (13) | −0.0254 (13) |
| C19 | 0.0511 (9) | 0.0468 (10) | 0.0441 (10) | −0.0031 (7) | −0.0004 (7) | −0.0015 (7) |
| C13 | 0.0499 (10) | 0.0543 (13) | 0.119 (2) | −0.0044 (9) | −0.0018 (11) | −0.0084 (12) |
| C12 | 0.0512 (9) | 0.0415 (11) | 0.0810 (14) | 0.0022 (7) | 0.0016 (9) | −0.0019 (9) |
| C15 | 0.0744 (13) | 0.0752 (16) | 0.0804 (14) | 0.0126 (11) | −0.0187 (11) | −0.0219 (12) |
| C11 | 0.0803 (14) | 0.0885 (18) | 0.119 (2) | −0.0205 (12) | 0.0373 (13) | 0.0061 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C2 | 1.3605 (19) | C16—H16 | 0.93 |
| O1—C1 | 1.409 (2) | C4—C5 | 1.374 (3) |
| O3—C9 | 1.339 (2) | C4—C3 | 1.378 (3) |
| O3—C10 | 1.440 (2) | C4—H4 | 0.93 |
| O2—C9 | 1.205 (2) | C3—C2 | 1.391 (2) |
| O6—C19 | 1.3370 (19) | C3—H3 | 0.93 |
| O6—C20 | 1.443 (2) | C5—C6 | 1.388 (3) |
| O4—C12 | 1.367 (2) | C5—H5 | 0.93 |
| O4—C11 | 1.436 (2) | C1—H1A | 0.96 |
| N3—C18 | 1.280 (2) | C1—H1B | 0.96 |
| N3—N4 | 1.3742 (17) | C1—H1C | 0.96 |
| O5—C19 | 1.1922 (19) | C20—H20A | 0.96 |
| N1—C8 | 1.281 (2) | C20—H20B | 0.96 |
| N1—N2 | 1.3846 (19) | C20—H20C | 0.96 |
| N2—C9 | 1.348 (2) | C10—H10A | 0.96 |
| N2—H2N | 0.86 | C10—H10B | 0.96 |
| N4—C19 | 1.353 (2) | C10—H10C | 0.96 |
| N4—H4N | 0.86 | C6—H6 | 0.93 |
| C7—C6 | 1.395 (2) | C14—C15 | 1.371 (3) |
| C7—C2 | 1.406 (2) | C14—C13 | 1.374 (3) |
| C7—C8 | 1.466 (2) | C14—H14 | 0.93 |
| C17—C16 | 1.386 (3) | C13—C12 | 1.396 (3) |
| C17—C12 | 1.403 (2) | C13—H13 | 0.93 |
| C17—C18 | 1.471 (2) | C15—H15 | 0.93 |
| C18—H18 | 0.93 | C11—H11A | 0.96 |
| C8—H8 | 0.93 | C11—H11B | 0.96 |
| C16—C15 | 1.379 (3) | C11—H11C | 0.96 |
| | | | |
| C2—O1—C1 | 118.57 (14) | O1—C1—H1C | 109.5 |
| C9—O3—C10 | 116.02 (15) | H1A—C1—H1C | 109.5 |

| | | | |
|---|---|---|---|
| C19—O6—C20 | 117.40 (15) | H1B—C1—H1C | 109.5 |
| C12—O4—C11 | 117.97 (16) | O1—C2—C3 | 123.94 (16) |
| C18—N3—N4 | 115.85 (13) | O1—C2—C7 | 115.33 (14) |
| C8—N1—N2 | 114.99 (13) | C3—C2—C7 | 120.73 (15) |
| C9—N2—N1 | 119.64 (13) | O6—C20—H20A | 109.5 |
| C9—N2—H2N | 120.2 | O6—C20—H20B | 109.5 |
| N1—N2—H2N | 120.2 | H20A—C20—H20B | 109.5 |
| C19—N4—N3 | 118.82 (13) | O6—C20—H20C | 109.5 |
| C19—N4—H4N | 120.6 | H20A—C20—H20C | 109.5 |
| N3—N4—H4N | 120.6 | H20B—C20—H20C | 109.5 |
| C6—C7—C2 | 117.76 (16) | O3—C10—H10A | 109.5 |
| C6—C7—C8 | 123.29 (16) | O3—C10—H10B | 109.5 |
| C2—C7—C8 | 118.96 (14) | H10A—C10—H10B | 109.5 |
| C16—C17—C12 | 118.26 (16) | O3—C10—H10C | 109.5 |
| C16—C17—C18 | 120.86 (16) | H10A—C10—H10C | 109.5 |
| C12—C17—C18 | 120.84 (16) | H10B—C10—H10C | 109.5 |
| N3—C18—C17 | 119.80 (15) | C5—C6—C7 | 121.06 (17) |
| N3—C18—H18 | 120.1 | C5—C6—H6 | 119.5 |
| C17—C18—H18 | 120.1 | C7—C6—H6 | 119.5 |
| N1—C8—C7 | 122.99 (15) | C15—C14—C13 | 120.82 (19) |
| N1—C8—H8 | 118.5 | C15—C14—H14 | 119.6 |
| C7—C8—H8 | 118.5 | C13—C14—H14 | 119.6 |
| O2—C9—O3 | 124.73 (16) | O5—C19—O6 | 124.49 (15) |
| O2—C9—N2 | 125.42 (16) | O5—C19—N4 | 126.70 (14) |
| O3—C9—N2 | 109.84 (14) | O6—C19—N4 | 108.79 (14) |
| C15—C16—C17 | 121.7 (2) | C14—C13—C12 | 120.1 (2) |
| C15—C16—H16 | 119.2 | C14—C13—H13 | 120.0 |
| C17—C16—H16 | 119.2 | C12—C13—H13 | 120.0 |
| C5—C4—C3 | 120.38 (18) | O4—C12—C13 | 124.25 (18) |
| C5—C4—H4 | 119.8 | O4—C12—C17 | 116.00 (15) |
| C3—C4—H4 | 119.8 | C13—C12—C17 | 119.75 (19) |
| C4—C3—C2 | 119.93 (17) | C14—C15—C16 | 119.4 (2) |
| C4—C3—H3 | 120.0 | C14—C15—H15 | 120.3 |
| C2—C3—H3 | 120.0 | C16—C15—H15 | 120.3 |
| C4—C5—C6 | 120.14 (17) | O4—C11—H11A | 109.5 |
| C4—C5—H5 | 119.9 | O4—C11—H11B | 109.5 |
| C6—C5—H5 | 119.9 | H11A—C11—H11B | 109.5 |
| O1—C1—H1A | 109.5 | O4—C11—H11C | 109.5 |
| O1—C1—H1B | 109.5 | H11A—C11—H11C | 109.5 |
| H1A—C1—H1B | 109.5 | H11B—C11—H11C | 109.5 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*N*···O5 | 0.86 | 2.08 | 2.938 (2) | 173 |
| N4—H4*N*···N1$^{i}$ | 0.86 | 2.42 | 3.279 (2) | 177 |

| | | | | |
|---|---|---|---|---|
| C1—H1*A*···O2$^{i}$ | 0.96 | 2.52 | 3.472 (2) | 170 |
| C11—H11*B*···*Cg*1$^{ii}$ | 0.96 | 2.87 | 3.826 (3) | 175 |

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