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# Di-*tert*-butyl 2-benzoylhydrazine-1,1-dicarboxylate

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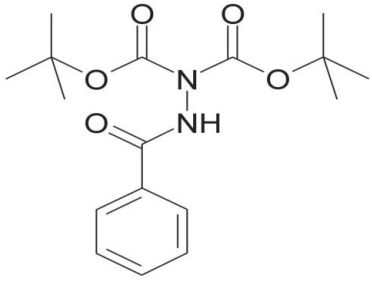
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.038; $wR$ factor = 0.109; data-to-parameter ratio = 8.6.

The crystal structure of the title compound, $C_{17}H_{24}N_2O_5$, was determined in the course of our studies on the preparation of two families of pseudopeptides, *viz*. hydrazino- and *N*-amino-peptides. The most significant interaction in the crystal structure is a bifurcated intermolecular N—H···O hydrogen bond.

## Related literature

For the synthesis, see: Brosse *et al.* (2003). For geometry, see: Allen (2002); Kauffmann *et al.* (2004); Fong *et al.* (1996).



## Experimental

### *Crystal data*

$C_{17}H_{24}N_2O_5$
$M_r$ = 336.38
Orthorhombic, $P2_12_12_1$
$a$ = 9.9794 (2) Å
$b$ = 11.5763 (3) Å
$c$ = 16.0720 (4) Å
$V$ = 1856.71 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 (2) K
0.3 × 0.05 × 0.05 mm

### *Data collection*

Nonius KappaCCD area-detector diffractometer
Absorption correction: none
9649 measured reflections
1944 independent reflections
1559 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.109
$S$ = 1.03
1944 reflections
226 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2···O2$^{i}$ | 0.82 (3) | 2.53 (3) | 3.233 (3) | 145 (3) |
| N2—H2···O4$^{i}$ | 0.82 (3) | 2.32 (3) | 3.062 (3) | 150 (3) |

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *WebLab ViewerPro 3.5* (MSI, 1999); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HJ2004).

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# supporting information

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## Di-*tert*-butyl 2-benzoylhydrazine-1,1-dicarboxylate

**Claude Didierjean, Nicolas Brosse, Jacques Bodiguel and Brigitte Jamart-Grégoire**

### S1. Comment

As part of our continuing studies on the synthesis and structure of hydrazino- and *N*-amino-peptides, we have described the crystal structure of *N*-(*tert*-Butyloxycarbonylamino)phthalimide (Kauffmann *et al.*, 2004). Here we report the crystal structure of the title compound, *N*-benzoyl-N$^{\beta}$, N$^{\alpha}$- bis (*tert*-butoxycarbonyl) hydrazine (Fig. 1).

Although the title compound is not chiral, it crystallizes in the non-centrosymmetric space group $P2_12_12_1$. The angle between the amide plane and the mean plane of the imidodicarbonate group is 78.43 (18)°, showing that these two groups are nearly perpendicular. The angle between the best-fit phenyl plane and the amide plane of 27.34 (7)° is similar to that reported for the benzamide group (Fong *et al.*, 1996).

In the crystal structure of the title compound, molecules are linked into infinite chains parallel to a *via* bifurcated N—H···O hydrogen bonds involving both carbonate of the aminoimidodicarbonate group (Fig. 2). All other intermolecular interactions are due to van der Waals forces.

### S2. Experimental

The title compound was prepared from *N*-(*tert*-Butyloxycarbonylamino)phthalimide (Brosse *et al.*, 2003), and was crystallized by slow evaporation of an ethanol solution.

### S3. Refinement

All H atoms were located in difference maps. The C-bonded H atoms were placed at calculated positions and refined using a riding model, with C—H distances of 0.93–0.96 Å. The N-bonded H atom was refined with free positional parameters. The H-atom $U_{iso}$ parameters were fixed at 1.3Ueq(C) for aromatic C—H groups, at 1.3Ueq(N) for the N—H group and at 1.5Ueq(C) for methyl C—H.

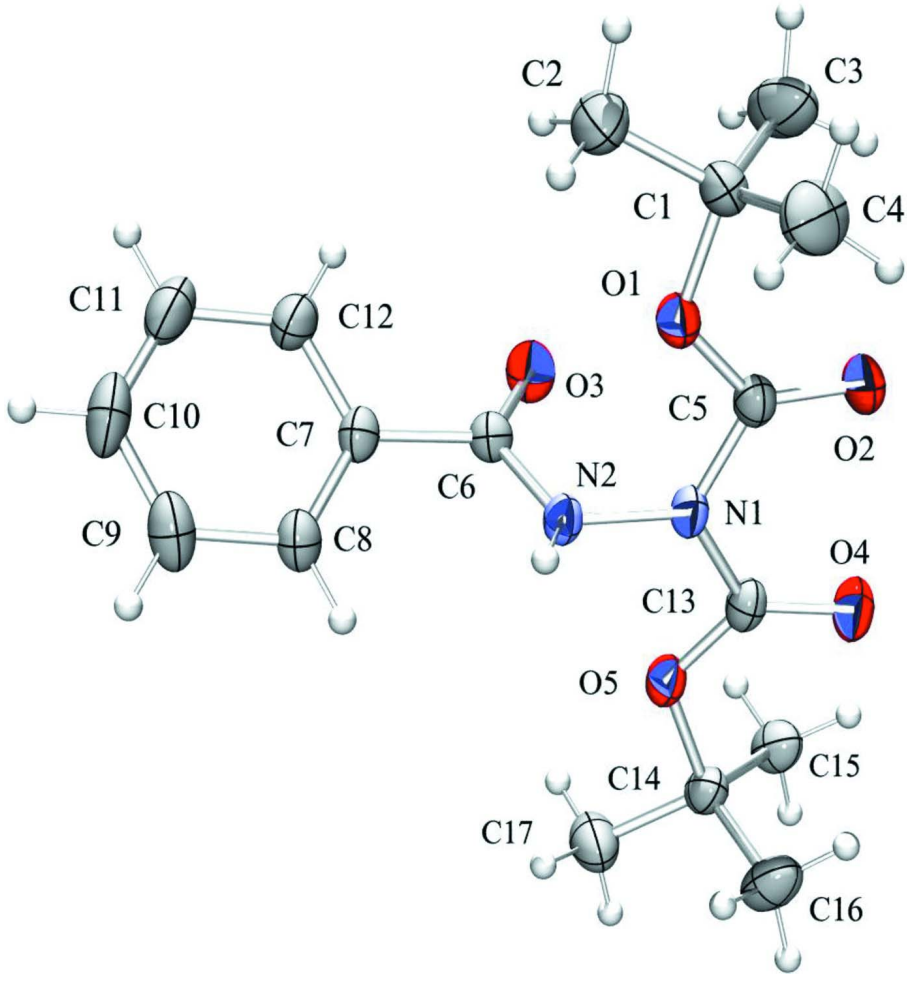


**Figure 1**

The molecular structure of title compound showing the atom-numbering scheme. All non-H atoms are represented by 25% probability displacement ellipsoids.

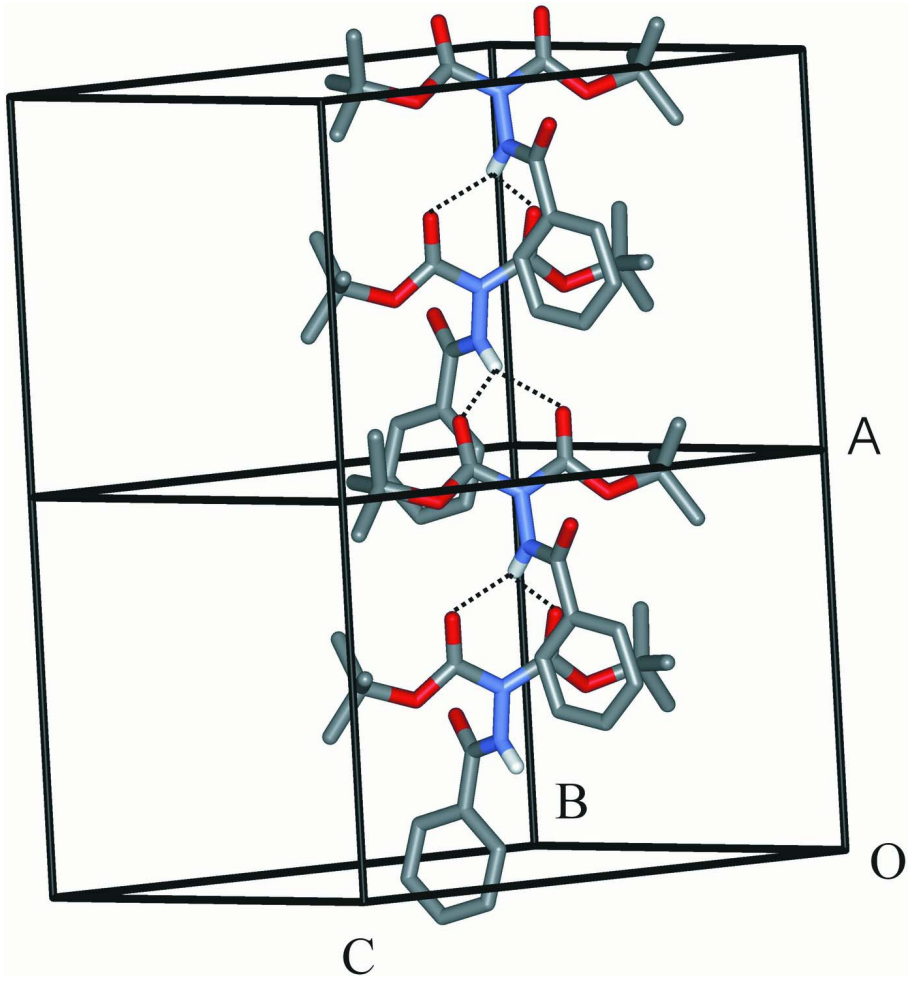


**Figure 2**

Part of the crystal structure of the title compound showing the chains along [100]. The intermolecular hydrogen bonds are shown as dashed lines.

## Di-*tert*-butyl 2-benzoylhydrazine-1,1-dicarboxylate

*Crystal data*

$C_{17}H_{24}N_2O_5$
$M_r = 336.38$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 9.9794\ (2)$ Å
$b = 11.5763\ (3)$ Å
$c = 16.0720\ (4)$ Å
$V = 1856.71\ (8)$ Å$^3$
$Z = 4$
$F(000) = 720$
$D_x = 1.203$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å
Cell parameters from 9649 reflections
$\theta = 2.5$–$25.5°$
$\mu = 0.09$ mm$^{-1}$
$T = 293$ K
Prism, colorless
0.3 × 0.05 × 0.05 mm

*Data collection*

Nonius KappaCCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scans
9649 measured reflections
1944 independent reflections
1559 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.032
$\theta_{max}$ = 25.5°, $\theta_{min}$ = 2.5°
$h$ = −11→11
$k$ = −14→14
$l$ = −19→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.109
$S$ = 1.03
1944 reflections
226 parameters
0 restraints
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2 + 0.077P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.044
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 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.

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.5100 (2) | −0.0209 (2) | −0.17416 (18) | 0.0659 (7) |
| C2 | 0.6320 (3) | 0.0439 (4) | −0.2024 (2) | 0.0978 (11) |
| H2A | 0.6566 | 0.0997 | −0.1609 | 0.147* |
| H2B | 0.6128 | 0.0829 | −0.2538 | 0.147* |
| H2C | 0.7046 | −0.0092 | −0.2106 | 0.147* |
| C3 | 0.3937 (3) | 0.0597 (3) | −0.1641 (3) | 0.1131 (13) |
| H3A | 0.3137 | 0.0158 | −0.154 | 0.17* |
| H3B | 0.3829 | 0.1045 | −0.2139 | 0.17* |
| H3C | 0.4099 | 0.1104 | −0.1179 | 0.17* |
| C4 | 0.4826 (5) | −0.1216 (4) | −0.2302 (2) | 0.1084 (12) |
| H4A | 0.5609 | −0.1695 | −0.2334 | 0.163* |
| H4B | 0.4602 | −0.094 | −0.2848 | 0.163* |
| H4C | 0.4092 | −0.1657 | −0.2084 | 0.163* |
| O1 | 0.55435 (15) | −0.06767 (16) | −0.09296 (11) | 0.0615 (5) |
| C5 | 0.4705 (2) | −0.1231 (2) | −0.04390 (17) | 0.0556 (6) |
| O2 | 0.35449 (18) | −0.14394 (19) | −0.05764 (15) | 0.0834 (6) |
| N1 | 0.53802 (19) | −0.15842 (17) | 0.02859 (13) | 0.0533 (5) |
| N2 | 0.67171 (18) | −0.12688 (16) | 0.03912 (13) | 0.0493 (5) |
| H2 | 0.723 (3) | −0.177 (2) | 0.0211 (18) | 0.064* |
| C6 | 0.7009 (2) | −0.0142 (2) | 0.05343 (15) | 0.0501 (6) |
| O3 | 0.61438 (18) | 0.05698 (16) | 0.06796 (13) | 0.0722 (5) |
| C7 | 0.8465 (2) | 0.0151 (2) | 0.04796 (15) | 0.0530 (6) |
| C8 | 0.9465 (2) | −0.0644 (2) | 0.06302 (17) | 0.0629 (7) |
| H8 | 0.9244 | −0.139 | 0.0795 | 0.082* |
| C9 | 1.0804 (3) | −0.0334 (3) | 0.0536 (2) | 0.0855 (10) |
| H9 | 1.1477 | −0.0872 | 0.0637 | 0.111* |
| C10 | 1.1127 (3) | 0.0761 (4) | 0.0296 (2) | 0.0952 (11) |

| | | | | |
|---|---|---|---|---|
| H10 | 1.2022 | 0.0965 | 0.0232 | 0.124* |
| C11 | 1.0149 (4) | 0.1561 (3) | 0.0149 (2) | 0.0937 (11) |
| H11 | 1.0378 | 0.2304 | −0.0019 | 0.122* |
| C12 | 0.8811 (3) | 0.1263 (3) | 0.02503 (19) | 0.0735 (8) |
| H12 | 0.8146 | 0.1812 | 0.0164 | 0.096* |
| C13 | 0.4706 (2) | −0.2161 (2) | 0.09331 (16) | 0.0542 (6) |
| O4 | 0.35904 (18) | −0.25409 (17) | 0.08502 (12) | 0.0743 (6) |
| O5 | 0.54681 (15) | −0.22196 (15) | 0.15998 (11) | 0.0584 (4) |
| C14 | 0.5017 (3) | −0.2927 (2) | 0.23280 (17) | 0.0595 (6) |
| C15 | 0.3708 (3) | −0.2462 (2) | 0.26688 (19) | 0.0715 (8) |
| H15A | 0.3791 | −0.1646 | 0.2764 | 0.107* |
| H15B | 0.3502 | −0.2843 | 0.3184 | 0.107* |
| H15C | 0.3003 | −0.2601 | 0.2275 | 0.107* |
| C16 | 0.4944 (3) | −0.4176 (3) | 0.2060 (2) | 0.0883 (10) |
| H16A | 0.423 | −0.427 | 0.1665 | 0.132* |
| H16B | 0.4778 | −0.4655 | 0.2536 | 0.132* |
| H16C | 0.5777 | −0.4396 | 0.1807 | 0.132* |
| C17 | 0.6120 (3) | −0.2720 (4) | 0.2951 (2) | 0.0920 (10) |
| H17A | 0.6962 | −0.2953 | 0.2717 | 0.138* |
| H17B | 0.5947 | −0.3162 | 0.3445 | 0.138* |
| H17C | 0.6153 | −0.1914 | 0.3089 | 0.138* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0554 (13) | 0.0720 (17) | 0.0704 (16) | −0.0016 (12) | −0.0099 (13) | 0.0087 (14) |
| C2 | 0.077 (2) | 0.125 (3) | 0.091 (2) | −0.022 (2) | −0.0004 (18) | 0.034 (2) |
| C3 | 0.080 (2) | 0.096 (2) | 0.163 (4) | 0.026 (2) | 0.012 (3) | 0.041 (3) |
| C4 | 0.137 (3) | 0.108 (3) | 0.080 (2) | −0.020 (3) | −0.023 (2) | −0.010 (2) |
| O1 | 0.0458 (8) | 0.0760 (11) | 0.0626 (10) | −0.0073 (9) | −0.0035 (8) | 0.0080 (9) |
| C5 | 0.0431 (13) | 0.0549 (13) | 0.0689 (16) | −0.0016 (11) | 0.0006 (12) | 0.0000 (12) |
| O2 | 0.0423 (10) | 0.1008 (14) | 0.1071 (16) | −0.0138 (9) | −0.0132 (10) | 0.0264 (13) |
| N1 | 0.0362 (10) | 0.0588 (11) | 0.0648 (12) | −0.0080 (8) | 0.0018 (9) | 0.0017 (10) |
| N2 | 0.0359 (10) | 0.0495 (11) | 0.0626 (12) | −0.0023 (8) | 0.0041 (9) | −0.0032 (9) |
| C6 | 0.0476 (13) | 0.0537 (13) | 0.0490 (13) | −0.0005 (10) | 0.0015 (11) | −0.0047 (11) |
| O3 | 0.0571 (10) | 0.0634 (10) | 0.0960 (13) | 0.0068 (9) | 0.0060 (9) | −0.0205 (11) |
| C7 | 0.0470 (12) | 0.0615 (14) | 0.0503 (13) | −0.0099 (11) | 0.0009 (11) | −0.0090 (11) |
| C8 | 0.0499 (13) | 0.0681 (15) | 0.0707 (16) | −0.0058 (13) | −0.0006 (12) | −0.0143 (14) |
| C9 | 0.0511 (15) | 0.106 (3) | 0.099 (2) | −0.0035 (16) | 0.0008 (16) | −0.032 (2) |
| C10 | 0.0616 (18) | 0.125 (3) | 0.099 (2) | −0.039 (2) | 0.0132 (18) | −0.022 (2) |
| C11 | 0.088 (2) | 0.096 (2) | 0.098 (3) | −0.042 (2) | 0.0036 (19) | 0.0067 (19) |
| C12 | 0.0696 (17) | 0.0702 (17) | 0.0806 (19) | −0.0189 (14) | −0.0040 (15) | 0.0049 (16) |
| C13 | 0.0439 (13) | 0.0551 (13) | 0.0637 (14) | −0.0060 (11) | 0.0075 (12) | −0.0056 (12) |
| O4 | 0.0537 (10) | 0.0951 (14) | 0.0740 (12) | −0.0262 (10) | 0.0028 (9) | −0.0005 (10) |
| O5 | 0.0451 (8) | 0.0669 (10) | 0.0632 (10) | −0.0113 (8) | 0.0039 (8) | 0.0058 (9) |
| C14 | 0.0508 (13) | 0.0568 (15) | 0.0711 (17) | −0.0038 (11) | 0.0058 (12) | 0.0078 (12) |
| C15 | 0.0632 (16) | 0.0717 (18) | 0.0796 (18) | 0.0039 (14) | 0.0190 (14) | 0.0056 (14) |
| C16 | 0.092 (2) | 0.0553 (17) | 0.118 (3) | 0.0054 (16) | 0.023 (2) | 0.0053 (16) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C17 | 0.0674 (17) | 0.123 (3) | 0.086 (2) | −0.0129 (19) | −0.0080 (17) | 0.027 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—O1 | 1.481 (3) | C8—C9 | 1.393 (4) |
| C1—C3 | 1.498 (4) | C8—H8 | 0.93 |
| C1—C4 | 1.498 (5) | C9—C10 | 1.363 (5) |
| C1—C2 | 1.500 (4) | C9—H9 | 0.93 |
| C2—H2A | 0.96 | C10—C11 | 1.367 (5) |
| C2—H2B | 0.96 | C10—H10 | 0.93 |
| C2—H2C | 0.96 | C11—C12 | 1.388 (4) |
| C3—H3A | 0.96 | C11—H11 | 0.93 |
| C3—H3B | 0.96 | C12—H12 | 0.93 |
| C3—H3C | 0.96 | C13—O4 | 1.204 (3) |
| C4—H4A | 0.96 | C13—O5 | 1.316 (3) |
| C4—H4B | 0.96 | O5—C14 | 1.498 (3) |
| C4—H4C | 0.96 | C14—C17 | 1.508 (4) |
| O1—C5 | 1.317 (3) | C14—C16 | 1.510 (4) |
| C5—O2 | 1.203 (3) | C14—C15 | 1.515 (4) |
| C5—N1 | 1.407 (3) | C15—H15A | 0.96 |
| N1—N2 | 1.393 (3) | C15—H15B | 0.96 |
| N1—C13 | 1.407 (3) | C15—H15C | 0.96 |
| N2—C6 | 1.356 (3) | C16—H16A | 0.96 |
| N2—H2 | 0.82 (3) | C16—H16B | 0.96 |
| C6—O3 | 1.216 (3) | C16—H16C | 0.96 |
| C6—C7 | 1.495 (3) | C17—H17A | 0.96 |
| C7—C8 | 1.378 (4) | C17—H17B | 0.96 |
| C7—C12 | 1.383 (4) | C17—H17C | 0.96 |
| | | | |
| O1—C1—C3 | 111.4 (3) | C9—C8—H8 | 119.9 |
| O1—C1—C4 | 107.5 (2) | C10—C9—C8 | 119.8 (3) |
| C3—C1—C4 | 114.0 (3) | C10—C9—H9 | 120.1 |
| O1—C1—C2 | 102.0 (2) | C8—C9—H9 | 120.1 |
| C3—C1—C2 | 110.5 (3) | C9—C10—C11 | 120.7 (3) |
| C4—C1—C2 | 110.8 (3) | C9—C10—H10 | 119.6 |
| C1—C2—H2A | 109.5 | C11—C10—H10 | 119.6 |
| C1—C2—H2B | 109.5 | C10—C11—C12 | 119.8 (3) |
| H2A—C2—H2B | 109.5 | C10—C11—H11 | 120.1 |
| C1—C2—H2C | 109.5 | C12—C11—H11 | 120.1 |
| H2A—C2—H2C | 109.5 | C7—C12—C11 | 120.2 (3) |
| H2B—C2—H2C | 109.5 | C7—C12—H12 | 119.9 |
| C1—C3—H3A | 109.5 | C11—C12—H12 | 119.9 |
| C1—C3—H3B | 109.5 | O4—C13—O5 | 127.3 (2) |
| H3A—C3—H3B | 109.5 | O4—C13—N1 | 122.3 (2) |
| C1—C3—H3C | 109.5 | O5—C13—N1 | 110.47 (18) |
| H3A—C3—H3C | 109.5 | C13—O5—C14 | 119.39 (17) |
| H3B—C3—H3C | 109.5 | O5—C14—C17 | 102.3 (2) |
| C1—C4—H4A | 109.5 | O5—C14—C16 | 108.3 (2) |

| | | | |
|---|---|---|---|
| C1—C4—H4B | 109.5 | C17—C14—C16 | 112.2 (3) |
| H4A—C4—H4B | 109.5 | O5—C14—C15 | 110.3 (2) |
| C1—C4—H4C | 109.5 | C17—C14—C15 | 109.4 (2) |
| H4A—C4—H4C | 109.5 | C16—C14—C15 | 113.7 (2) |
| H4B—C4—H4C | 109.5 | C14—C15—H15A | 109.5 |
| C5—O1—C1 | 121.07 (18) | C14—C15—H15B | 109.5 |
| O2—C5—O1 | 126.8 (3) | H15A—C15—H15B | 109.5 |
| O2—C5—N1 | 123.7 (2) | C14—C15—H15C | 109.5 |
| O1—C5—N1 | 109.43 (19) | H15A—C15—H15C | 109.5 |
| N2—N1—C5 | 118.9 (2) | H15B—C15—H15C | 109.5 |
| N2—N1—C13 | 119.5 (2) | C14—C16—H16A | 109.5 |
| C5—N1—C13 | 121.37 (19) | C14—C16—H16B | 109.5 |
| C6—N2—N1 | 118.55 (19) | H16A—C16—H16B | 109.5 |
| C6—N2—H2 | 127.0 (19) | C14—C16—H16C | 109.5 |
| N1—N2—H2 | 111.5 (19) | H16A—C16—H16C | 109.5 |
| O3—C6—N2 | 122.2 (2) | H16B—C16—H16C | 109.5 |
| O3—C6—C7 | 123.2 (2) | C14—C17—H17A | 109.5 |
| N2—C6—C7 | 114.6 (2) | C14—C17—H17B | 109.5 |
| C8—C7—C12 | 119.1 (2) | H17A—C17—H17B | 109.5 |
| C8—C7—C6 | 122.8 (2) | C14—C17—H17C | 109.5 |
| C12—C7—C6 | 118.0 (2) | H17A—C17—H17C | 109.5 |
| C7—C8—C9 | 120.2 (3) | H17B—C17—H17C | 109.5 |
| C7—C8—H8 | 119.9 | | |

| | | | |
|---|---|---|---|
| C3—C1—O1—C5 | 56.4 (3) | C12—C7—C8—C9 | −1.3 (4) |
| C4—C1—O1—C5 | −69.2 (3) | C6—C7—C8—C9 | 177.3 (3) |
| C2—C1—O1—C5 | 174.2 (3) | C7—C8—C9—C10 | 0.2 (5) |
| C1—O1—C5—O2 | 1.2 (4) | C8—C9—C10—C11 | 0.2 (5) |
| C1—O1—C5—N1 | 179.81 (19) | C9—C10—C11—C12 | 0.5 (6) |
| O2—C5—N1—N2 | −178.3 (2) | C8—C7—C12—C11 | 2.0 (4) |
| O1—C5—N1—N2 | 3.1 (3) | C6—C7—C12—C11 | −176.7 (3) |
| O2—C5—N1—C13 | −3.7 (4) | C10—C11—C12—C7 | −1.6 (5) |
| O1—C5—N1—C13 | 177.6 (2) | N2—N1—C13—O4 | −173.4 (2) |
| C5—N1—N2—C6 | 69.7 (3) | C5—N1—C13—O4 | 12.0 (4) |
| C13—N1—N2—C6 | −105.0 (3) | N2—N1—C13—O5 | 5.8 (3) |
| N1—N2—C6—O3 | 9.7 (4) | C5—N1—C13—O5 | −168.72 (19) |
| N1—N2—C6—C7 | −169.0 (2) | O4—C13—O5—C14 | 6.9 (4) |
| O3—C6—C7—C8 | 154.6 (3) | N1—C13—O5—C14 | −172.37 (19) |
| N2—C6—C7—C8 | −26.7 (4) | C13—O5—C14—C17 | −177.6 (2) |
| O3—C6—C7—C12 | −26.7 (4) | C13—O5—C14—C16 | 63.8 (3) |
| N2—C6—C7—C12 | 151.9 (2) | C13—O5—C14—C15 | −61.3 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O2$^{i}$ | 0.82 (3) | 2.53 (3) | 3.233 (3) | 145 (3) |

| | | | | |
|---|---|---|---|---|
| N2—H2···O4$^{i}$ | 0.82 (3) | 2.32 (3) | 3.062 (3) | 150 (3) |

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