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# Methyl *N*-{(1*R*)-2-[(methoxycarbonyl)oxy]-1-phenylethyl}carbamate

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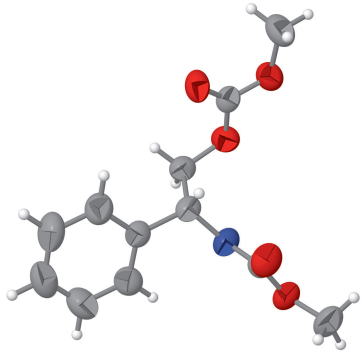
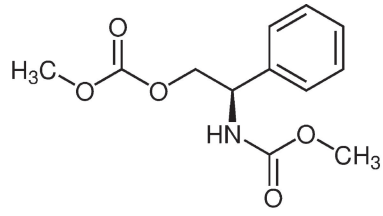
**Structural data:** full structural data are available from iucrdata.iucr.org

The title molecule, $C_{12}H_{15}NO_5$, is a methyl carbamate derivative obtained by reacting (*R*)-2-phenylglycinol and methyl chloroformate, with calcium hydroxide as heterogeneous catalyst. Supramolecular chains are formed in the [100] direction, based on N—H···O hydrogen bonds between the amide and carboxylate groups. These chains weakly interact in the crystal, and the phenyl rings do not display significant $\pi$–$\pi$ interactions.

3D view



Chemical scheme




## Structure description

Methyl carbamate, $Me(O)CONH_2$, the methyl ester of carbamic acid, is an important intermediate in the manufacture of carbamate-based resins used in the textile and polymer industries. On a smaller scale, it is also a pharmaceutical intermediate. The primary amine group can be functionalized, in the same way as for primary amides. From another point of view, the formation of a carbamate *via* a *N*-methyloxycarbonylation reaction can also be considered as a useful protection of a primary amine (Sartori *et al.*, 2004). Finally, alternative routes allow both the formation of the carbamate and the *N*-functionalization. The title compound, $C_{12}H_{15}NO_5$, resulted from such a reaction, between methyl chloroformate and a chiral amino alcohol, namely (*R*)-2-phenylglycinol, under basic conditions, and using $Ca(OH)_2$ as a heterogeneous catalyst.

We assumed that the *R* absolute configuration of the starting material was retained during the reaction, affording an enantiomerically pure compound, which crystallized in the Sohncke space group $P2_12_12_1$. Molecular dimensions are as expected, and the amide group displays a geometry quite different from that of the carboxylate group, with bond lengths C2—N1 = 1.333 (3) and C10—O3 = 1.445 (3) Å (Fig. 1). The geometry of the

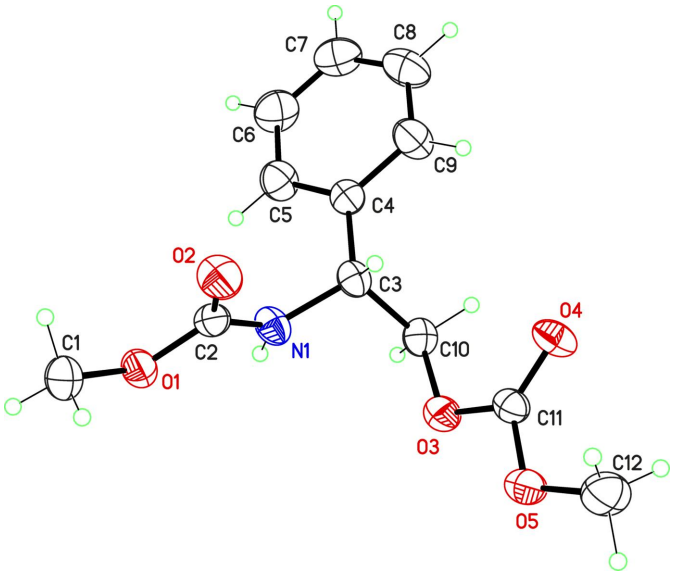



**Figure 1**
The molecular structure of the title compound (50% probability ellipsoids).

carbamate group is virtually identical to that observed in the closely related chiral compound methyl(1*S*-phenylethyl) carbamate, which crystallizes with four independent molecules in the asymmetric unit (Thakar *et al.*, 2018).

In the extended structure, the amide NH group serves as a donor, forming an intermolecular hydrogen bond with the carboxylate group C11═O4 of a neighbouring molecule (Table 1). Infinite chains are then formed in the crystal, running along the short *a* axis (Fig. 2). Molecules are further connected through weak C—H···O contacts involving the methyl group of the carbamate moiety as donor. Chains are

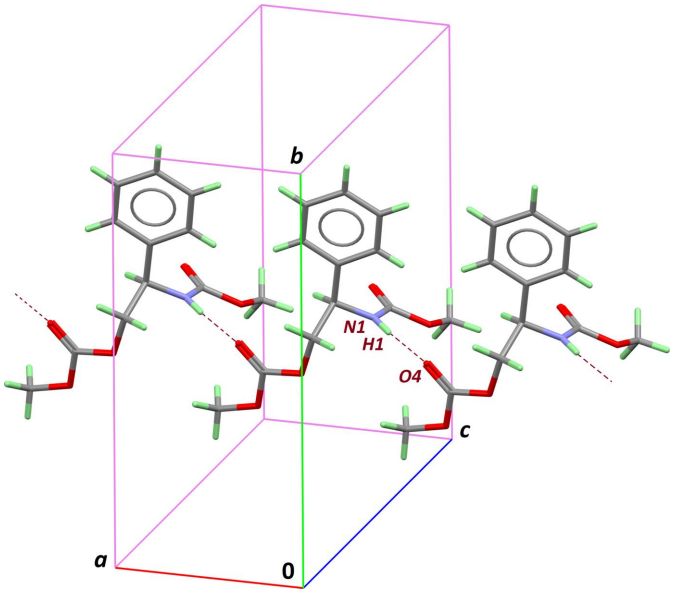



**Figure 2**
Supramolecular chains formed in the [100] direction, based on amide–carboxylate N—H···O hydrogen bonds (dashed bonds).

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O4$^{i}$ | 0.82 (3) | 2.10 (3) | 2.917 (2) | 175 (2) |
| C1—H1*B*···O4$^{ii}$ | 0.96 | 2.59 | 3.494 (3) | 158 |
| C1—H1*C*···O5$^{iii}$ | 0.96 | 2.62 | 3.332 (4) | 131 |

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

arranged in the crystal with two neighbouring chains having the phenyl rings facing upwards (Fig. 3). However, no significant $\pi$–$\pi$ contacts are observed: the distance separating two rings is large [4.6763 (17) Å] and the dihedral angle between corresponding mean planes is 21.84 (13)°. Aside from the weak C—H···O bonds mentioned above and van der Waals contacts, no other significant interactions between the supramolecular chains are present in the crystal structure. As a consequence, the Kitaigorodskii packing index of 67.8% is rather low for this small organic molecule (Spek, 2020).

## Synthesis and crystallization

(*R*)-2-Phenylglycinol (100 mg, 0.73 mmol) was dissolved in dry THF. The catalyst, $Ca(OH)_2$ (10%), and methyl chloroformate (0.56 ml, 7.2 mmol) were added, and the mixture was refluxed (333 K) under a nitrogen atmosphere. After completion (TLC), the catalyst was separated by filtration, and the crude product recovered by elimination of the solvent under reduced pressure. The crude product was recrystallized from a mixture of solvents (hexane:$CH_2Cl_2$, 4:1 *v*:*v*), affording single crystals suitable for X-ray diffraction. $^{1}$H-NMR (500 MHz, $CDCl_3$): $\delta$ 3.66 (*s*, 3H), 3.76 (*s*, 3H), 4.35 (*s*, 2H), 5.05 (*broad*, 1H), 5.64 (*broad*, 1H), 7.29–7.37 (*m*, 5H) p.p.m. $^{13}$C-NMR (126 MHz, $CDCl_3$): $\delta$ 52.33, 54.2, 55.06, 69.66, 126.59, 128.06, 128.80, 138.20, 155.68, 156.41 p.p.m.

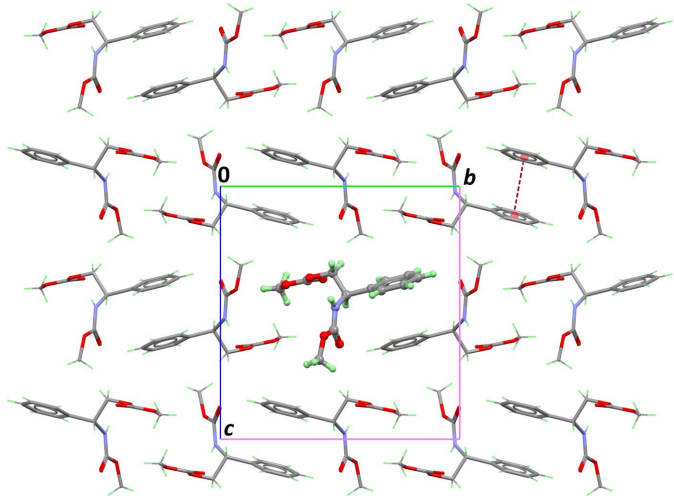



**Figure 3**
Part of the crystal structure of the title compound, viewed down the crystallographic *a* axis. The asymmetric unit is shown as a ball and stick model, and the dashed line represents the weak $\pi$–$\pi$ interaction between phenyl rings.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The amide H atom (H1) was refined with free coordinates and isotropic displacement parameter. Other H atoms are in calculated positions. The absolute configuration was inferred from the synthesis.


## Acknowledgements

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**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{12}H_{15}NO_5$ |
| $M_r$ | 253.25 |
| Crystal system, space group | Orthorhombic, $P2_12_12_1$ |
| Temperature (K) | 295 |
| $a, b, c$ (Å) | 6.2497 (2), 13.8633 (6), 14.6254 (5) |
| $V$ (Å$^3$) | 1267.17 (8) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.10 |
| Crystal size (mm) | 0.67 × 0.29 × 0.16 |
| | |
| Data collection | |
| Diffractometer | Xcalibur, Atlas, Gemini |
| Absorption correction | Multi-scan (*CrysAlis PRO*; Rigaku OD, 2022) |
| $T_{min}$, $T_{max}$ | 0.967, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 24119, 3859, 2841 |
| $R_{int}$ | 0.035 |
| $(\sin\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.714 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.046, 0.118, 1.03 |
| No. of reflections | 3859 |
| No. of parameters | 169 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.14, −0.16 |

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *XP* in *SHELXTL-Plus* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

# full crystallographic data

*IUCrData* (2024). **9**, x240222 [https://doi.org/10.1107/S2414314624002220]

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**Methyl *N*-{(1*R*)-2-[(methoxycarbonyl)oxy]-1-phenylethyl}carbamate**

*Crystal data*

$C_{12}H_{15}NO_5$
$M_r$ = 253.25
Orthorhombic, $P2_12_12_1$
$a$ = 6.2497 (2) Å
$b$ = 13.8633 (6) Å
$c$ = 14.6254 (5) Å
$V$ = 1267.17 (8) Å$^3$
$Z$ = 4
$F(000)$ = 536
$D_x$ = 1.327 Mg m$^{-3}$
Melting point: 345 K
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4907 reflections
$\theta$ = 3.3–26.1°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 295 K
Block, colourless
0.67 × 0.29 × 0.16 mm

*Data collection*

Xcalibur, Atlas, Gemini diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.5564 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)
$T_{min}$ = 0.967, $T_{max}$ = 1.000
24119 measured reflections
3859 independent reflections
2841 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035
$\theta_{max}$ = 30.5°, $\theta_{min}$ = 2.9°
$h$ = −8→8
$k$ = −19→19
$l$ = −20→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.118
$S$ = 1.03
3859 reflections
169 parameters
0 restraints
0 constraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.052P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | −0.2085 (3) | 0.43365 (12) | 0.59140 (10) | 0.0598 (4) |
| O2 | 0.1160 (3) | 0.49818 (13) | 0.62348 (10) | 0.0670 (5) |

| | | | | |
|---|---|---|---|---|
| O3 | 0.2905 (2) | 0.37368 (12) | 0.36207 (12) | 0.0607 (4) |
| O4 | 0.6279 (2) | 0.42897 (11) | 0.36564 (11) | 0.0597 (4) |
| O5 | 0.5449 (3) | 0.27357 (12) | 0.38930 (13) | 0.0668 (5) |
| N1 | −0.0043 (3) | 0.48073 (14) | 0.47814 (11) | 0.0527 (4) |
| H1 | −0.105 (4) | 0.4625 (18) | 0.4474 (16) | 0.053 (6)* |
| C1 | −0.2419 (5) | 0.4127 (2) | 0.68630 (17) | 0.0769 (8) |
| H1A | −0.387398 | 0.392701 | 0.695569 | 0.115* |
| H1B | −0.213777 | 0.469417 | 0.721969 | 0.115* |
| H1C | −0.147035 | 0.361905 | 0.704931 | 0.115* |
| C2 | −0.0183 (3) | 0.47379 (15) | 0.56885 (13) | 0.0475 (4) |
| C3 | 0.1699 (3) | 0.52669 (16) | 0.43010 (13) | 0.0473 (5) |
| H3 | 0.297760 | 0.524175 | 0.468833 | 0.057* |
| C4 | 0.1259 (4) | 0.63165 (16) | 0.40547 (13) | 0.0492 (5) |
| C5 | −0.0757 (4) | 0.6723 (2) | 0.41155 (19) | 0.0678 (7) |
| H5 | −0.190104 | 0.634538 | 0.430815 | 0.081* |
| C6 | −0.1102 (5) | 0.7682 (2) | 0.3895 (2) | 0.0834 (8) |
| H6 | −0.246934 | 0.794183 | 0.394150 | 0.100* |
| C7 | 0.0544 (6) | 0.8242 (2) | 0.36108 (19) | 0.0790 (8) |
| H7 | 0.030618 | 0.888693 | 0.346652 | 0.095* |
| C8 | 0.2556 (6) | 0.7862 (2) | 0.3536 (2) | 0.0868 (9) |
| H8 | 0.368411 | 0.824713 | 0.333876 | 0.104* |
| C9 | 0.2916 (5) | 0.6898 (2) | 0.37548 (19) | 0.0725 (7) |
| H9 | 0.428547 | 0.664215 | 0.369869 | 0.087* |
| C10 | 0.2142 (4) | 0.46992 (18) | 0.34271 (14) | 0.0541 (5) |
| H10A | 0.083947 | 0.465903 | 0.306877 | 0.065* |
| H10B | 0.320390 | 0.503898 | 0.306596 | 0.065* |
| C11 | 0.5013 (4) | 0.36477 (15) | 0.37178 (13) | 0.0492 (4) |
| C12 | 0.7676 (4) | 0.2503 (2) | 0.4027 (2) | 0.0787 (8) |
| H12A | 0.850042 | 0.275381 | 0.352705 | 0.118* |
| H12B | 0.784356 | 0.181520 | 0.405485 | 0.118* |
| H12C | 0.816598 | 0.278478 | 0.458896 | 0.118* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0627 (9) | 0.0623 (9) | 0.0543 (8) | −0.0127 (8) | 0.0094 (7) | −0.0026 (7) |
| O2 | 0.0727 (10) | 0.0791 (12) | 0.0492 (8) | −0.0157 (9) | −0.0091 (8) | −0.0040 (8) |
| O3 | 0.0484 (8) | 0.0545 (9) | 0.0791 (10) | −0.0078 (7) | 0.0020 (8) | −0.0061 (8) |
| O4 | 0.0521 (8) | 0.0539 (9) | 0.0732 (10) | −0.0146 (7) | −0.0156 (8) | 0.0141 (8) |
| O5 | 0.0597 (9) | 0.0467 (9) | 0.0940 (12) | −0.0059 (7) | 0.0045 (8) | 0.0026 (8) |
| N1 | 0.0464 (9) | 0.0661 (11) | 0.0457 (9) | −0.0137 (9) | −0.0059 (8) | 0.0020 (8) |
| C1 | 0.098 (2) | 0.0742 (19) | 0.0583 (13) | −0.0119 (15) | 0.0262 (14) | −0.0041 (12) |
| C2 | 0.0533 (11) | 0.0412 (10) | 0.0479 (10) | 0.0005 (9) | −0.0004 (9) | −0.0013 (8) |
| C3 | 0.0395 (9) | 0.0585 (12) | 0.0439 (9) | −0.0055 (9) | −0.0062 (7) | 0.0019 (8) |
| C4 | 0.0512 (11) | 0.0560 (12) | 0.0403 (9) | −0.0038 (10) | −0.0048 (9) | −0.0002 (9) |
| C5 | 0.0576 (14) | 0.0716 (17) | 0.0742 (15) | 0.0022 (12) | −0.0028 (11) | 0.0071 (14) |
| C6 | 0.0823 (19) | 0.0727 (19) | 0.095 (2) | 0.0178 (16) | −0.0093 (17) | 0.0056 (15) |
| C7 | 0.107 (3) | 0.0602 (15) | 0.0697 (16) | 0.0062 (16) | −0.0161 (15) | 0.0083 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.102 (2) | 0.069 (2) | 0.0893 (19) | −0.0242 (17) | −0.0026 (18) | 0.0189 (15) |
| C9 | 0.0614 (14) | 0.0686 (16) | 0.0873 (17) | −0.0081 (12) | 0.0014 (14) | 0.0136 (14) |
| C10 | 0.0488 (10) | 0.0626 (14) | 0.0508 (10) | 0.0009 (10) | −0.0021 (9) | 0.0004 (10) |
| C11 | 0.0524 (11) | 0.0489 (11) | 0.0464 (10) | −0.0090 (10) | −0.0008 (10) | −0.0009 (9) |
| C12 | 0.0703 (16) | 0.0606 (16) | 0.105 (2) | 0.0071 (12) | −0.0097 (17) | 0.0120 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C2 | 1.353 (3) | C4—C5 | 1.383 (3) |
| O1—C1 | 1.433 (3) | C4—C9 | 1.384 (3) |
| O2—C2 | 1.207 (2) | C5—C6 | 1.385 (4) |
| O3—C11 | 1.331 (3) | C5—H5 | 0.9300 |
| O3—C10 | 1.445 (3) | C6—C7 | 1.355 (4) |
| O4—C11 | 1.194 (2) | C6—H6 | 0.9300 |
| O5—C11 | 1.318 (3) | C7—C8 | 1.368 (5) |
| O5—C12 | 1.442 (3) | C7—H7 | 0.9300 |
| N1—C2 | 1.333 (3) | C8—C9 | 1.392 (4) |
| N1—C3 | 1.444 (3) | C8—H8 | 0.9300 |
| N1—H1 | 0.82 (3) | C9—H9 | 0.9300 |
| C1—H1A | 0.9600 | C10—H10A | 0.9700 |
| C1—H1B | 0.9600 | C10—H10B | 0.9700 |
| C1—H1C | 0.9600 | C12—H12A | 0.9600 |
| C3—C4 | 1.524 (3) | C12—H12B | 0.9600 |
| C3—C10 | 1.526 (3) | C12—H12C | 0.9600 |
| C3—H3 | 0.9800 | | |
| | | | |
| C2—O1—C1 | 116.6 (2) | C7—C6—C5 | 120.3 (3) |
| C11—O3—C10 | 115.66 (17) | C7—C6—H6 | 119.9 |
| C11—O5—C12 | 116.11 (19) | C5—C6—H6 | 119.9 |
| C2—N1—C3 | 124.45 (18) | C6—C7—C8 | 120.1 (3) |
| C2—N1—H1 | 118.4 (17) | C6—C7—H7 | 120.0 |
| C3—N1—H1 | 116.9 (17) | C8—C7—H7 | 120.0 |
| O1—C1—H1A | 109.5 | C7—C8—C9 | 120.0 (3) |
| O1—C1—H1B | 109.5 | C7—C8—H8 | 120.0 |
| H1A—C1—H1B | 109.5 | C9—C8—H8 | 120.0 |
| O1—C1—H1C | 109.5 | C4—C9—C8 | 120.7 (3) |
| H1A—C1—H1C | 109.5 | C4—C9—H9 | 119.6 |
| H1B—C1—H1C | 109.5 | C8—C9—H9 | 119.6 |
| O2—C2—N1 | 126.4 (2) | O3—C10—C3 | 111.83 (17) |
| O2—C2—O1 | 124.37 (19) | O3—C10—H10A | 109.2 |
| N1—C2—O1 | 109.27 (18) | C3—C10—H10A | 109.2 |
| N1—C3—C4 | 113.60 (18) | O3—C10—H10B | 109.2 |
| N1—C3—C10 | 108.46 (18) | C3—C10—H10B | 109.2 |
| C4—C3—C10 | 109.09 (17) | H10A—C10—H10B | 107.9 |
| N1—C3—H3 | 108.5 | O4—C11—O5 | 126.4 (2) |
| C4—C3—H3 | 108.5 | O4—C11—O3 | 125.3 (2) |
| C10—C3—H3 | 108.5 | O5—C11—O3 | 108.30 (18) |
| C5—C4—C9 | 117.7 (2) | O5—C12—H12A | 109.5 |

| | | | |
|---|---|---|---|
| C5—C4—C3 | 122.6 (2) | O5—C12—H12B | 109.5 |
| C9—C4—C3 | 119.8 (2) | H12A—C12—H12B | 109.5 |
| C4—C5—C6 | 121.2 (3) | O5—C12—H12C | 109.5 |
| C4—C5—H5 | 119.4 | H12A—C12—H12C | 109.5 |
| C6—C5—H5 | 119.4 | H12B—C12—H12C | 109.5 |
| | | | |
| C3—N1—C2—O2 | −5.4 (4) | C5—C6—C7—C8 | 0.4 (5) |
| C3—N1—C2—O1 | 175.16 (19) | C6—C7—C8—C9 | −0.2 (5) |
| C1—O1—C2—O2 | −5.0 (3) | C5—C4—C9—C8 | 0.9 (4) |
| C1—O1—C2—N1 | 174.4 (2) | C3—C4—C9—C8 | −179.3 (2) |
| C2—N1—C3—C4 | −95.0 (2) | C7—C8—C9—C4 | −0.4 (5) |
| C2—N1—C3—C10 | 143.5 (2) | C11—O3—C10—C3 | −88.4 (2) |
| N1—C3—C4—C5 | −12.6 (3) | N1—C3—C10—O3 | −65.0 (2) |
| C10—C3—C4—C5 | 108.5 (2) | C4—C3—C10—O3 | 170.79 (16) |
| N1—C3—C4—C9 | 167.6 (2) | C12—O5—C11—O4 | 0.4 (4) |
| C10—C3—C4—C9 | −71.3 (3) | C12—O5—C11—O3 | −179.5 (2) |
| C9—C4—C5—C6 | −0.8 (4) | C10—O3—C11—O4 | −0.1 (3) |
| C3—C4—C5—C6 | 179.4 (2) | C10—O3—C11—O5 | 179.81 (17) |
| C4—C5—C6—C7 | 0.2 (5) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O4$^{i}$ | 0.82 (3) | 2.10 (3) | 2.917 (2) | 175 (2) |
| C1—H1*B*···O4$^{ii}$ | 0.96 | 2.59 | 3.494 (3) | 158 |
| C1—H1*C*···O5$^{iii}$ | 0.96 | 2.62 | 3.332 (4) | 131 |

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