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# *trans*-4-(1-Naphthyl)-2-oxo-1,3-oxazolidine-5-carboxylic acid

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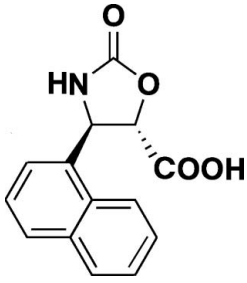
Key indicators: single-crystal X-ray study; $T$ = 292 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.037; $wR$ factor = 0.093; data-to-parameter ratio = 12.7.

The crystal structure of the title compound, $C_{14}H_{11}NO_4$, is influenced by N—H···O and O—H···O hydrogen bonds, linking molecules into one-dimensional tapes running along the [010] direction.

## Related literature

For general backgroud regarding the title compound, see: Lu *et al.* (2008). For patterns in hydrogen bonding, see: Bernstein *et al.* (1995). For related literature, see: Barbachyn & Ford (2003); Evans (1982); Mukhtar & Wright (2005).




## Experimental

### Crystal data

$C_{14}H_{11}NO_4$
$M_r$ = 257.24
Orthorhombic, *Pbca*
$a$ = 8.7159 (17) Å
$b$ = 12.817 (3) Å
$c$ = 20.737 (4) Å
$V$ = 2316.6 (8) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 292 (2) K
0.47 × 0.38 × 0.35 mm

### Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
12484 measured reflections
2266 independent reflections
2008 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.016

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.093
$S$ = 1.04
2266 reflections
178 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···O4$^{i}$ | 0.94 (2) | 1.72 (2) | 2.6591 (15) | 174 (2) |
| N1—H1···O2$^{ii}$ | 0.834 (17) | 2.247 (17) | 3.0097 (18) | 152.0 (15) |

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, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

We thank Dr Xiang-Gao Meng for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2191).

## References

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# supporting information

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## *trans*-4-(1-Naphthyl)-2-oxo-1,3-oxazolidine-5-carboxylic acid

**Jiao-Yan Yang, Zhi-Hui Ming, Jing An, Qiu-Lin Hua and Liang-Qiu Lu**

### S1. Comment

Oxazolidin-2-ones are prevalent in biologically active molecules (Mukhtar *et al.*, 2005; Barbachyn, *et al.*, 2003), as well as versatile synthons in organic synthesis (Evans, 1982). Recently we reported a new cascade reaction to synthesize these compounds from stable sulfur ylides and nitroolefins (Lu *et al.*, 2008). In order to demostrate the utility of this method we continued to hydrolyze *trans*-ethyl 4-(naphthalen-1-yl)-2-oxooxazolidine-5-carboxylate with LiOH to obtain *trans*-4-(naphthalen-1-yl)-2-oxooxazolidine-5-carboxylic acid, and we are presenting herein the X-ray crystallographic analysis of the title compound, thus obtained (Fig. 1),

The crystal structure is determined by N—H···O and O—H···O hydrogen bonds, defining $R_2^2(8)$ rings (Bernstein *et al.* (1995), which link molecules into one-dimensional hydrogen-bonded tapes along [010] ( Fig. 2).

### S2. Experimental

The starting material, 4-(naphthalen-1-yl)-2-oxooxazolidine-5-carboxylate (100.0 mg, 0.35 mmol) was added to the aqueous solution of LiOH (88.1 mg, 2.10 mmol, 2.5 ml H2O) and the reaction mixture was stirred for 2.5 h. By adjusting the pH = 6–7 with concentrated HCl and 1*M* diluted HCl solution, the white solid precipitated and was filtrated. The residue was washed with cold water and diethyl ester, the desired product was collected as white power after dryness with 93% yield. Recrystallization from CH3OH—H2O provided the crystalline solid.

### S3. Refinement

All H atoms bonded to C atoms were initially located in difference Fourier maps and then constrained to their ideal geometry positions with C–H=0.96Å (methyl), 0.97Å (methylene). H atoms bonded to N and O were found in difference maps and refined with N/O—H distances free. In all cases $U_{iso}$ ((H) values were set to x times $U_{eq}$(host), x= 1.5(methyl), x=1.2 (methylene), x=1.2 (N), x=1.5 (O).

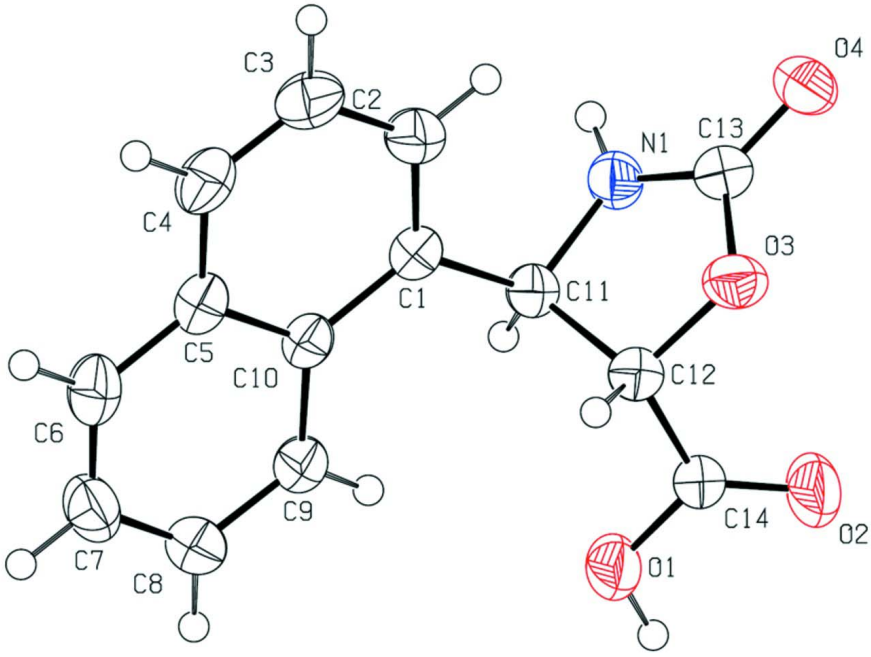


**Figure 1**

View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

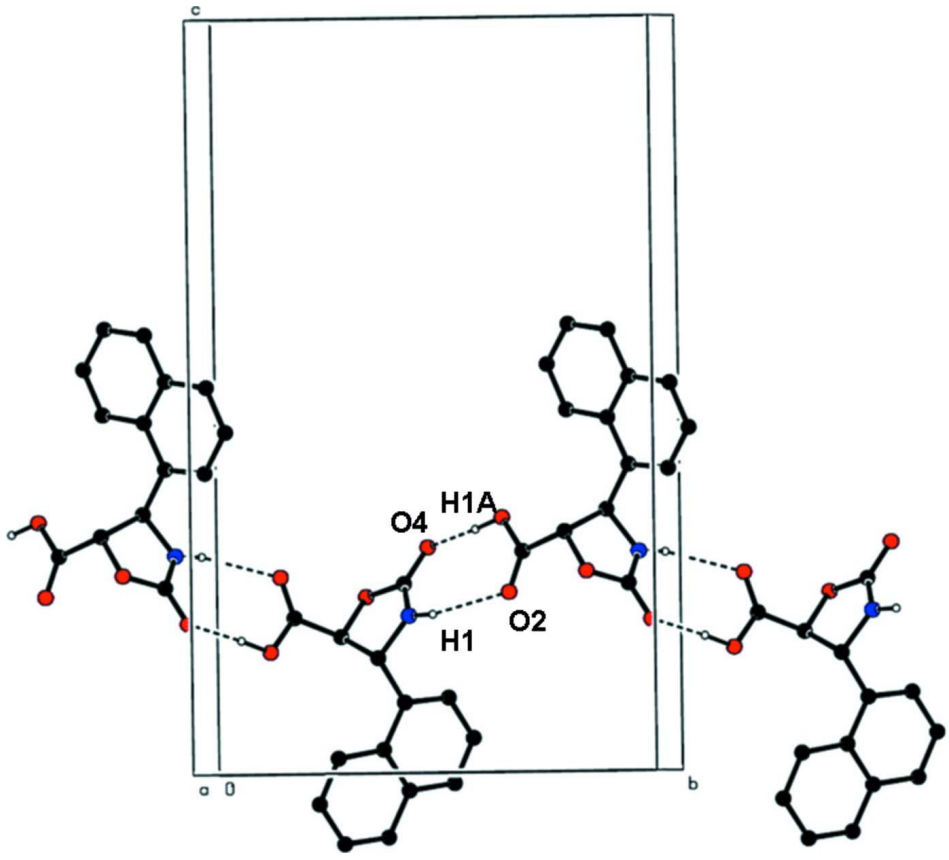


**Figure 2**

Packing of (I) with hydrogen bonds drawn as dashed lines showing the formation of hydrogen-bonded $R_2^2(8)$ loops involving NH···O and OH···O hydrogen bonds. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry codes: (i) -*x*, *y* - 1/2, -*z* + 1/2; (ii) -*x*, *y* + 1/2, *z* + 1/2]

### *trans*-4-(1-Naphthyl)-2-oxo-1,3-oxazolidine-5-carboxylic acid

*Crystal data*

$C_{14}H_{11}NO_4$
$M_r$ = 257.24
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
*a* = 8.7159 (17) Å
*b* = 12.817 (3) Å
*c* = 20.737 (4) Å
*V* = 2316.6 (8) Å$^3$
*Z* = 8
*F*(000) = 1072
$D_x$ = 1.475 Mg m$^{-3}$
Mo *Kα* radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5223 reflections
$\theta$ = 2.8–28.9°
$\mu$ = 0.11 mm$^{-1}$
*T* = 292 K
Block, colorless
0.47 × 0.38 × 0.35 mm

*Data collection*

Bruker SMART 4K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
12484 measured reflections
2266 independent reflections
2008 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.016
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 3.0°
*h* = −9→10
*k* = −15→15
*l* = −25→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.093$
$S = 1.05$
2266 reflections
178 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2 + 0.7823P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å$^{-3}$
$\Delta\rho_{min} = -0.20$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.10060 (15) | 0.89669 (10) | 0.40612 (6) | 0.0322 (3) |
| C2 | 0.18399 (17) | 0.98662 (11) | 0.40013 (7) | 0.0415 (3) |
| H2 | 0.1971 | 1.0159 | 0.3595 | 0.050* |
| C3 | 0.25014 (19) | 1.03567 (11) | 0.45381 (7) | 0.0474 (4) |
| H3 | 0.3063 | 1.0967 | 0.4484 | 0.057* |
| C4 | 0.23264 (17) | 0.99464 (12) | 0.51357 (7) | 0.0438 (4) |
| H4 | 0.2764 | 1.0280 | 0.5489 | 0.053* |
| C5 | 0.14847 (15) | 0.90147 (11) | 0.52271 (6) | 0.0363 (3) |
| C6 | 0.13034 (17) | 0.85684 (12) | 0.58449 (7) | 0.0435 (4) |
| H6 | 0.1731 | 0.8900 | 0.6201 | 0.052* |
| C7 | 0.05170 (18) | 0.76650 (13) | 0.59291 (7) | 0.0468 (4) |
| H7 | 0.0424 | 0.7377 | 0.6339 | 0.056* |
| C8 | −0.01545 (17) | 0.71659 (12) | 0.53978 (7) | 0.0435 (3) |
| H8 | −0.0694 | 0.6548 | 0.5458 | 0.052* |
| C9 | −0.00239 (15) | 0.75784 (10) | 0.47936 (6) | 0.0359 (3) |
| H9 | −0.0490 | 0.7242 | 0.4448 | 0.043* |
| C10 | 0.08091 (14) | 0.85104 (10) | 0.46843 (6) | 0.0315 (3) |
| C11 | 0.03291 (15) | 0.84401 (10) | 0.34692 (6) | 0.0326 (3) |
| H11 | −0.0684 | 0.8149 | 0.3567 | 0.039* |
| C12 | 0.13968 (15) | 0.75872 (10) | 0.31821 (6) | 0.0356 (3) |
| H12 | 0.2150 | 0.7374 | 0.3507 | 0.043* |
| C13 | 0.13627 (16) | 0.89576 (10) | 0.24897 (7) | 0.0370 (3) |
| C14 | 0.05709 (17) | 0.66298 (10) | 0.29259 (6) | 0.0390 (3) |
| N1 | 0.02505 (13) | 0.91215 (9) | 0.29122 (5) | 0.0363 (3) |

| | | | | |
|---|---|---|---|---|
| H1 | −0.0281 (18) | 0.9662 (13) | 0.2897 (7) | 0.044* |
| O1 | −0.01994 (14) | 0.61525 (9) | 0.33777 (5) | 0.0538 (3) |
| H1A | −0.068 (3) | 0.5549 (17) | 0.3222 (10) | 0.081* |
| O2 | 0.0653 (2) | 0.63355 (10) | 0.23870 (5) | 0.0869 (5) |
| O3 | 0.21709 (11) | 0.80945 (7) | 0.26568 (5) | 0.0429 (3) |
| O4 | 0.17042 (13) | 0.94603 (8) | 0.20100 (5) | 0.0497 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0341 (6) | 0.0298 (6) | 0.0328 (7) | 0.0010 (5) | 0.0002 (5) | −0.0034 (5) |
| C2 | 0.0503 (8) | 0.0350 (7) | 0.0394 (7) | −0.0056 (6) | 0.0002 (6) | 0.0012 (6) |
| C3 | 0.0529 (9) | 0.0346 (8) | 0.0545 (9) | −0.0125 (6) | −0.0010 (7) | −0.0056 (6) |
| C4 | 0.0452 (8) | 0.0422 (8) | 0.0439 (8) | −0.0054 (6) | −0.0044 (6) | −0.0138 (6) |
| C5 | 0.0358 (7) | 0.0378 (7) | 0.0353 (7) | 0.0037 (6) | −0.0010 (5) | −0.0071 (6) |
| C6 | 0.0452 (8) | 0.0538 (9) | 0.0316 (7) | 0.0033 (7) | −0.0036 (6) | −0.0071 (6) |
| C7 | 0.0544 (9) | 0.0542 (9) | 0.0319 (7) | 0.0063 (7) | 0.0019 (6) | 0.0065 (6) |
| C8 | 0.0505 (8) | 0.0383 (8) | 0.0415 (8) | −0.0020 (6) | 0.0059 (6) | 0.0035 (6) |
| C9 | 0.0402 (7) | 0.0339 (7) | 0.0337 (7) | −0.0017 (6) | 0.0008 (5) | −0.0038 (5) |
| C10 | 0.0322 (6) | 0.0306 (6) | 0.0317 (6) | 0.0032 (5) | 0.0004 (5) | −0.0042 (5) |
| C11 | 0.0363 (7) | 0.0314 (7) | 0.0302 (6) | −0.0008 (5) | −0.0008 (5) | −0.0002 (5) |
| C12 | 0.0421 (7) | 0.0314 (7) | 0.0333 (7) | 0.0010 (6) | 0.0005 (6) | 0.0009 (5) |
| C13 | 0.0407 (7) | 0.0313 (7) | 0.0389 (7) | 0.0004 (6) | 0.0004 (6) | 0.0004 (6) |
| C14 | 0.0563 (9) | 0.0307 (7) | 0.0301 (7) | −0.0004 (6) | 0.0037 (6) | −0.0003 (5) |
| N1 | 0.0398 (6) | 0.0369 (6) | 0.0322 (6) | 0.0083 (5) | 0.0001 (5) | 0.0023 (5) |
| O1 | 0.0767 (8) | 0.0478 (6) | 0.0370 (6) | −0.0233 (6) | 0.0127 (5) | −0.0085 (5) |
| O2 | 0.1626 (15) | 0.0612 (8) | 0.0371 (6) | −0.0509 (9) | 0.0266 (8) | −0.0154 (6) |
| O3 | 0.0437 (5) | 0.0328 (5) | 0.0521 (6) | 0.0043 (4) | 0.0128 (5) | 0.0052 (4) |
| O4 | 0.0620 (7) | 0.0415 (6) | 0.0457 (6) | 0.0059 (5) | 0.0143 (5) | 0.0106 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.3682 (19) | C8—H8 | 0.9300 |
| C1—C10 | 1.4289 (17) | C9—C10 | 1.4160 (18) |
| C1—C11 | 1.5202 (17) | C9—H9 | 0.9300 |
| C2—C3 | 1.403 (2) | C11—N1 | 1.4497 (16) |
| C2—H2 | 0.9300 | C11—C12 | 1.5542 (18) |
| C3—C4 | 1.355 (2) | C11—H11 | 0.9800 |
| C3—H3 | 0.9300 | C12—O3 | 1.4368 (16) |
| C4—C5 | 1.414 (2) | C12—C14 | 1.5185 (19) |
| C4—H4 | 0.9300 | C12—H12 | 0.9800 |
| C5—C6 | 1.4117 (19) | C13—O4 | 1.2220 (16) |
| C5—C10 | 1.4253 (18) | C13—N1 | 1.3233 (18) |
| C6—C7 | 1.357 (2) | C13—O3 | 1.3565 (16) |
| C6—H6 | 0.9300 | C14—O2 | 1.1817 (17) |
| C7—C8 | 1.402 (2) | C14—O1 | 1.3049 (17) |
| C7—H7 | 0.9300 | N1—H1 | 0.834 (17) |
| C8—C9 | 1.3647 (19) | O1—H1A | 0.94 (2) |

| | | | |
|---|---|---|---|
| C2—C1—C10 | 119.40 (12) | C9—C10—C5 | 117.90 (12) |
| C2—C1—C11 | 120.46 (12) | C9—C10—C1 | 123.49 (11) |
| C10—C1—C11 | 120.12 (11) | C5—C10—C1 | 118.61 (12) |
| C1—C2—C3 | 121.59 (13) | N1—C11—C1 | 113.21 (11) |
| C1—C2—H2 | 119.2 | N1—C11—C12 | 98.44 (10) |
| C3—C2—H2 | 119.2 | C1—C11—C12 | 112.92 (11) |
| C4—C3—C2 | 120.38 (13) | N1—C11—H11 | 110.6 |
| C4—C3—H3 | 119.8 | C1—C11—H11 | 110.6 |
| C2—C3—H3 | 119.8 | C12—C11—H11 | 110.6 |
| C3—C4—C5 | 120.58 (13) | O3—C12—C14 | 108.85 (10) |
| C3—C4—H4 | 119.7 | O3—C12—C11 | 104.67 (10) |
| C5—C4—H4 | 119.7 | C14—C12—C11 | 114.74 (11) |
| C6—C5—C4 | 121.45 (13) | O3—C12—H12 | 109.5 |
| C6—C5—C10 | 119.12 (13) | C14—C12—H12 | 109.5 |
| C4—C5—C10 | 119.43 (12) | C11—C12—H12 | 109.5 |
| C7—C6—C5 | 121.27 (13) | O4—C13—N1 | 129.31 (13) |
| C7—C6—H6 | 119.4 | O4—C13—O3 | 120.76 (12) |
| C5—C6—H6 | 119.4 | N1—C13—O3 | 109.92 (12) |
| C6—C7—C8 | 119.93 (13) | O2—C14—O1 | 124.10 (14) |
| C6—C7—H7 | 120.0 | O2—C14—C12 | 124.05 (13) |
| C8—C7—H7 | 120.0 | O1—C14—C12 | 111.81 (11) |
| C9—C8—C7 | 120.66 (14) | C13—N1—C11 | 113.40 (11) |
| C9—C8—H8 | 119.7 | C13—N1—H1 | 120.9 (11) |
| C7—C8—H8 | 119.7 | C11—N1—H1 | 123.9 (11) |
| C8—C9—C10 | 121.10 (12) | C14—O1—H1A | 111.7 (13) |
| C8—C9—H9 | 119.5 | C13—O3—C12 | 108.59 (10) |
| C10—C9—H9 | 119.5 | | |

| | | | |
|---|---|---|---|
| C10—C1—C2—C3 | −0.4 (2) | C2—C1—C11—N1 | −17.73 (18) |
| C11—C1—C2—C3 | −178.76 (13) | C10—C1—C11—N1 | 163.91 (11) |
| C1—C2—C3—C4 | 0.0 (2) | C2—C1—C11—C12 | 93.05 (15) |
| C2—C3—C4—C5 | 0.4 (2) | C10—C1—C11—C12 | −85.31 (14) |
| C3—C4—C5—C6 | 179.30 (15) | N1—C11—C12—O3 | 21.29 (12) |
| C3—C4—C5—C10 | −0.4 (2) | C1—C11—C12—O3 | −98.41 (12) |
| C4—C5—C6—C7 | −178.87 (14) | N1—C11—C12—C14 | −97.95 (12) |
| C10—C5—C6—C7 | 0.8 (2) | C1—C11—C12—C14 | 142.36 (11) |
| C5—C6—C7—C8 | −1.0 (2) | O3—C12—C14—O2 | 4.2 (2) |
| C6—C7—C8—C9 | 0.1 (2) | C11—C12—C14—O2 | 121.12 (18) |
| C7—C8—C9—C10 | 0.9 (2) | O3—C12—C14—O1 | −177.87 (12) |
| C8—C9—C10—C5 | −1.09 (19) | C11—C12—C14—O1 | −61.00 (16) |
| C8—C9—C10—C1 | 178.86 (13) | O4—C13—N1—C11 | −171.98 (14) |
| C6—C5—C10—C9 | 0.22 (19) | O3—C13—N1—C11 | 7.85 (16) |
| C4—C5—C10—C9 | 179.92 (12) | C1—C11—N1—C13 | 101.23 (13) |
| C6—C5—C10—C1 | −179.73 (12) | C12—C11—N1—C13 | −18.24 (14) |
| C4—C5—C10—C1 | −0.03 (19) | O4—C13—O3—C12 | −172.25 (13) |
| C2—C1—C10—C9 | −179.53 (13) | N1—C13—O3—C12 | 7.90 (15) |
| C11—C1—C10—C9 | −1.16 (19) | C14—C12—O3—C13 | 104.23 (12) |

| | | | |
|---|---|---|---|
| C2—C1—C10—C5 | 0.42 (19) | C11—C12—O3—C13 | −18.91 (13) |
| C11—C1—C10—C5 | 178.79 (11) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*A*···O4$^{i}$ | 0.94 (2) | 1.72 (2) | 2.6591 (15) | 174 (2) |
| N1—H1···O2$^{ii}$ | 0.834 (17) | 2.247 (17) | 3.0097 (18) | 152.0 (15) |

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