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(2*S*)-4-Methyl-2-(1-oxo-1*H*-2,3-dihydro-isoindol-2-yl)pentanoic acid

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The title compound, $C_{14}H_{17}NO_3$, exhibits carboxylic acid group disorder about the $C-CO_2$ axis, with site occupancies of 0.79 (5):0.21 (5). Molecules are linked by intermolecular $O-H\cdots O{=}C_{iso}$, $C-H\cdots O{=}C_{iso}$ and $C-H\cdots\pi$(arene) interactions (iso = isoindolinone).

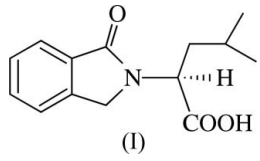
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.044
wR factor = 0.080
Data-to-parameter ratio = 7.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The majority of structurally determined phthalimidine systems are either *N*-substituted or have a hydroxy substituent at the 3-position (McNab *et al.*, 1997; Mukherjee *et al.*, 2000). The title compound, (I), synthesized from L-leucine and *ortho*-phthalaldehyde (Allin *et al.*, 1996), forms part of a structural study of phthalimidines (Brady *et al.*, 1998; Gallagher *et al.*, 2000; Gallagher & Brady, 2000; Gallagher & Murphy, 2001).



(I)

The molecular structure of (I) is depicted in Fig. 1 (*S* configuration) and selected dimensions are given in Table 1. The geometric data are normal (McNab *et al.*, 1997) and in agreement with expected values (Allen, 2002). The five- and six-membered rings of the isoindole group are coplanar [dihedral angle between rings = 1.0 (2)°], and the isoindolinone atom O3 is 0.022 (5) Å from the C_4N ring plane; this ring is oriented at 82.5 (5)° to the major orientation of the CCO_2 plane (O1*A*/O2*A*/C1/C2).

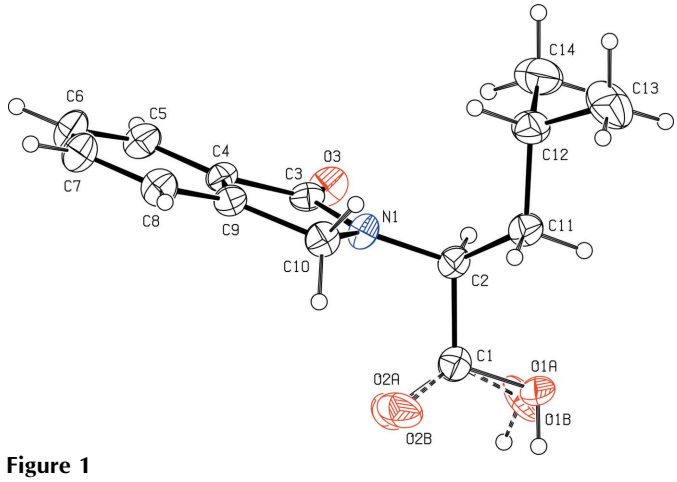


Figure 1
A view of (I), with the atomic numbering scheme; displacement ellipsoids are drawn at the 30% probability level. Both disorder components are shown.

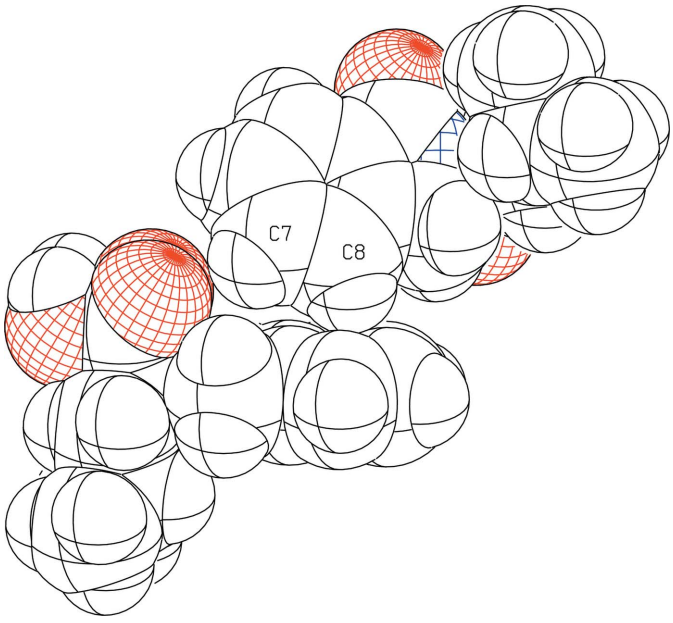


Figure 2
Two molecules of (I), with atoms depicted as their van der Waals spheres, with C7 (C—H···O^{iii} contact) and C8 [C—H···π(arene)^{iii}] labels.

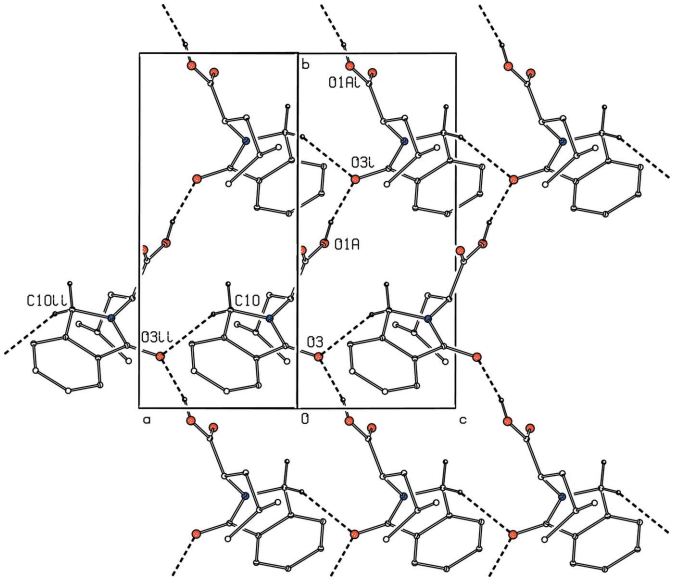


Figure 3
A view of the $C(7)C(5)[R_4^3(20)]$ sheet in (I) with the unit-cell outline (symmetry codes as in Table 2); H atoms not involved in hydrogen bonding have been omitted for clarity.

Molecules of (I) exhibit CO_2H group disorder about the C—CO_2 axis with site occupancies of 0.79 (5):0.21 (5) for the major/minor sites, respectively. Conventional CO_2H dimeric hydrogen bonding [$R_2^2(8)$ ring] is not present as a requirement of symmetry; rather, the primary hydrogen bonding as an $(\cdots O—H\cdots O—H\cdots)_n$ chain along [010] involving O1*A*/*B*—H1*A*/*B*···O3^{i} (Table 1) is described by a $C(7)$ motif (Grell *et al.*, 1999). The closest H atoms to the carbonyl O2*A*/*B* are at contact distances, *e.g.* H7···O2*A*^{iii} is 2.71 Å, with C7—H7···O2*A*^{iii} = 136° (symmetry codes iii as in Table 2). Disorder is facilitated on geometric grounds as O2 can rotate about the C1—C2 axis without greatly affecting the O1*A*/*B*—H1*A*/*B*···O3^{i} interaction distance (Fig. 2).

Combination of the O—H···O=C_{iso} $C(7)$ motif with a $C(5)$ motif (from C10—H10*A*···O3^{ii}) generates a two-dimensional sheet comprising $R_4^3(20)$ rings as $C(7)C(5)[R_4^3(20)]$; modest (arene)C—H···π(arene) interactions (Nishio, 2004) link these sheets (Fig. 3 and Table 2).

Compound (I) and the L-norvaline derivative, (II), $C_{13}H_{15}NO_3$, (2*S*)-2-(1-oxo-1*H*-2,3-dihydroisoindol-2-yl)-pentanoic acid (Gallagher & Brady, 2000), both crystallize in space group $P2_12_12_1$ with similar cell dimensions. The corresponding atom coordinates and molecular conformations are comparable and hence the crystal structures are isomorphous. Molecules of (I) and (II) differ in their respective alkyl chains with the $(CH_3)_2CHCH_2$– group in (I) occupying a similar volume as the disordered $CH_3CH_2CH_2$– group in (II). The solid-state (KBr disk) C=O stretching vibrations are similar, 1736, 1638 cm^{-1} in (I) and 1730, 1649 cm^{-1} in (II), highlighting the analogous environments of both C=O groups in (I) and (II).

Experimental

The title compound (I) was prepared by the overnight reaction of L-leucine and *o*-phthalaldehyde in refluxing CH_3CN under N_2 (Allin *et al.*, 1996). Filtration of the hot solution and subsequent slow cooling of the filtrate allowed the isolation of block-like colourless crystals. M.p. 485–487 K (uncorrected).

Crystal data

$C_{14}H_{17}NO_3$
M_r = 247.29
Orthorhombic, $P2_12_12_1$
a = 5.8790 (5) Å
b = 12.5223 (16) Å
c = 18.029 (3) Å
V = 1327.3 (3) Å^3
Z = 4
D_x = 1.237 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (1) K
Block, colourless
0.35 × 0.25 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: none
2394 measured reflections
1373 independent reflections
889 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 25.0°
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.080
S = 1.00
1373 reflections
185 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0312P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.013 (2)

Table 1
Selected torsion angles (°).

C3—N1—C2—C11	133.9 (3)	O3—C3—N1—C2	−1.6 (5)
C3—N1—C2—C1	−97.4 (4)	O1*A*—C1—C2—C11	−51.2 (9)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1A—H1A···O3^{i}	0.82	1.83	2.634 (9)	168
C10—H10A···O3^{ii}	0.97	2.54	3.366 (4)	144
C8—H8···$Cg1^{iii}$	0.93	2.74	3.473 (4)	137
C2—H2···O3	0.98	2.38	2.812 (4)	106

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x+1, y, z$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$.

In the absence of significant anomalous dispersion effects, Friedel equivalents were merged prior to the final refinement cycles. The absolute configuration can be inferred from the known absolute configuration of the L-leucine starting material. H atoms were treated as riding atoms using the *SHELXL97* (Sheldrick, 1997) defaults [at 294 (1) K], with C—H distances from 0.93 to 0.98 Å and O—H = 0.82 Å, and with U_{iso}(H) from 1.2 to 1.5 times U_{eq}(C,O).

Data collection: *CAD-4* (Enraf–Nonius, 1992); cell refinement: *SET4* and *CELDIM* (Enraf–Nonius, 1992); data reduction: *DATRD2* in *NRCVAX96* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *NRCVAX96* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *WORDPERFECT* macro *PREP8* (Ferguson, 1998).

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supporting information

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Crystal data

$C_{14}H_{17}NO_3$
$M_r = 247.29$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.8790$ (5) Å
$b = 12.5223$ (16) Å
$c = 18.029$ (3) Å
$V = 1327.3$ (3) Å^3
$Z = 4$
$F(000) = 528$
IR ($\nu_{C=O}$, cm^{-1}): 1736, 1638 (KBr).
$D_x = 1.237$ Mg m^{-3}
Melting point: 486 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 15.0$–$25.0°$
$\mu = 0.09$ mm^{-1}
$T = 294$ K
Block, colourless
0.35 × 0.25 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: X-ray tube
Graphite monochromator
ω–2θ scans
2394 measured reflections
1373 independent reflections
889 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
$h = -6 \rightarrow 6$
$k = -14 \rightarrow 14$
$l = -21 \rightarrow 21$
3 standard reflections every 120 min
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.080$
$S = 1.00$
1373 reflections
185 parameters
36 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
$w = 1/[\sigma^2(F_o^2) + (0.0312P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.013 (2)

Special details

Experimental. ? #Insert any special details here.
Geometry. Mean plane data ex-*SHELXL97* for molecule (I) ##########
As detailed in the comment text section.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1A	0.648 (3)	0.4641 (5)	0.8185 (5)	0.059 (3)	0.79 (5)
O2A	0.667 (4)	0.4445 (9)	0.6954 (4)	0.074 (3)	0.79 (5)
O1B	0.582 (8)	0.459 (3)	0.807 (2)	0.059 (10)	0.21 (5)
O2B	0.752 (8)	0.458 (3)	0.7002 (18)	0.066 (10)	0.21 (5)
O3	0.5705 (4)	0.14460 (18)	0.70543 (13)	0.0517 (8)	
N1	0.8834 (5)	0.2520 (2)	0.70881 (13)	0.0380 (7)	
C1	0.7067 (7)	0.4140 (3)	0.75684 (19)	0.0457 (10)	
C2	0.8176 (6)	0.3080 (2)	0.77582 (16)	0.0392 (9)	
C3	0.7532 (6)	0.1753 (2)	0.67839 (18)	0.0371 (9)	
C4	0.8679 (6)	0.1403 (2)	0.61054 (17)	0.0370 (9)	
C5	0.8039 (7)	0.0641 (3)	0.55912 (18)	0.0527 (11)	
C6	0.9450 (8)	0.0476 (3)	0.4992 (2)	0.0605 (12)	
C7	1.1438 (8)	0.1045 (3)	0.4917 (2)	0.0593 (11)	
C8	1.2086 (6)	0.1802 (3)	0.54341 (18)	0.0495 (10)	
C9	1.0656 (6)	0.1982 (3)	0.60280 (17)	0.0387 (9)	
C10	1.0864 (6)	0.2761 (2)	0.66548 (17)	0.0432 (9)	
C11	1.0083 (7)	0.3177 (3)	0.83211 (19)	0.0481 (10)	
C12	1.1179 (8)	0.2129 (3)	0.8559 (2)	0.0552 (11)	
C13	1.2949 (8)	0.2351 (4)	0.9156 (2)	0.0842 (15)	
C14	0.9461 (8)	0.1313 (3)	0.8821 (2)	0.0753 (13)	
H1A	0.5976	0.5234	0.8082	0.071*	0.79 (5)
H2A	0.4770	0.4909	0.7871	0.071*	0.21 (5)
H2	0.6993	0.2643	0.7993	0.047*	
H5	0.6701	0.0253	0.5648	0.063*	
H6	0.9054	−0.0026	0.4635	0.073*	
H7	1.2367	0.0917	0.4509	0.071*	
H8	1.3442	0.2178	0.5383	0.059*	
H10A	1.2239	0.2640	0.6940	0.052*	
H10B	1.0850	0.3492	0.6477	0.052*	
H11A	0.9490	0.3530	0.8759	0.058*	
H11B	1.1256	0.3634	0.8114	0.058*	
H12	1.1970	0.1830	0.8128	0.066*	
H13A	1.4020	0.2869	0.8977	0.126*	
H13B	1.3735	0.1702	0.9276	0.126*	
H13C	1.2209	0.2622	0.9592	0.126*	
H14A	0.8369	0.1185	0.8436	0.113*	
H14B	0.8697	0.1578	0.9254	0.113*	
H14C	1.0228	0.0658	0.8940	0.113*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.079 (6)	0.047 (3)	0.051 (3)	0.035 (3)	−0.012 (4)	−0.008 (3)
O2A	0.103 (8)	0.075 (4)	0.044 (3)	0.039 (4)	−0.002 (3)	0.006 (3)
O1B	0.045 (16)	0.102 (17)	0.031 (11)	0.004 (12)	0.013 (12)	0.028 (11)

O2B	0.076 (16)	0.061 (11)	0.062 (13)	0.013 (11)	0.025 (10)	0.027 (10)
O3	0.0407 (17)	0.0489 (15)	0.0655 (17)	−0.0112 (14)	0.0112 (15)	−0.0048 (13)
N1	0.0326 (17)	0.0406 (15)	0.0408 (16)	−0.0046 (16)	0.0052 (15)	−0.0090 (14)
C1	0.049 (3)	0.045 (2)	0.043 (2)	0.001 (2)	0.002 (2)	−0.003 (2)
C2	0.039 (2)	0.0374 (19)	0.0408 (18)	0.000 (2)	0.0040 (19)	−0.0032 (17)
C3	0.035 (2)	0.0294 (18)	0.047 (2)	−0.0018 (19)	−0.0004 (19)	0.0021 (16)
C4	0.040 (2)	0.0315 (17)	0.0400 (18)	0.005 (2)	0.002 (2)	−0.0026 (16)
C5	0.059 (3)	0.040 (2)	0.059 (2)	−0.001 (2)	0.001 (2)	−0.0060 (19)
C6	0.074 (3)	0.052 (2)	0.055 (3)	0.007 (3)	0.002 (3)	−0.020 (2)
C7	0.067 (3)	0.060 (2)	0.051 (2)	0.015 (3)	0.011 (2)	−0.010 (2)
C8	0.041 (2)	0.056 (2)	0.051 (2)	0.003 (2)	0.008 (2)	−0.001 (2)
C9	0.037 (2)	0.0373 (19)	0.0418 (19)	0.003 (2)	0.0011 (19)	−0.0009 (17)
C10	0.038 (2)	0.044 (2)	0.0479 (19)	−0.007 (2)	−0.002 (2)	−0.0012 (16)
C11	0.051 (3)	0.045 (2)	0.048 (2)	0.009 (2)	−0.002 (2)	−0.0040 (18)
C12	0.059 (3)	0.054 (2)	0.053 (2)	0.019 (3)	0.005 (2)	0.0045 (19)
C13	0.062 (3)	0.117 (4)	0.073 (3)	0.021 (3)	−0.019 (3)	0.015 (3)
C14	0.083 (3)	0.062 (3)	0.081 (3)	0.011 (3)	0.006 (3)	0.018 (2)

Geometric parameters (Å, º)

O1A—C1	1.323 (7)	O2B—C1	1.193 (19)
O2A—C1	1.194 (7)	O1A—H1A	0.8200
O3—C3	1.241 (4)	O1B—H2A	0.8200
N1—C2	1.449 (4)	C2—H2	0.9800
N1—C3	1.345 (4)	C5—H5	0.9300
N1—C10	1.458 (4)	C6—H6	0.9300
C1—C2	1.518 (4)	C7—H7	0.9300
C2—C11	1.517 (4)	C8—H8	0.9300
C3—C4	1.464 (4)	C10—H10A	0.9700
C4—C9	1.377 (5)	C10—H10B	0.9700
C4—C5	1.383 (4)	C11—H11A	0.9700
C5—C6	1.377 (5)	C11—H11B	0.9700
C6—C7	1.375 (5)	C12—H12	0.9800
C7—C8	1.384 (4)	C13—H13A	0.9600
C8—C9	1.380 (4)	C13—H13B	0.9600
C9—C10	1.498 (4)	C13—H13C	0.9600
C11—C12	1.524 (4)	C14—H14A	0.9600
C12—C14	1.513 (5)	C14—H14B	0.9600
C12—C13	1.523 (5)	C14—H14C	0.9600
O1B—C1	1.292 (19)		
C2—N1—C3	122.2 (3)	C1—C2—H2	106.3
C2—N1—C10	124.4 (3)	C6—C5—H5	121.1
C3—N1—C10	113.3 (3)	C4—C5—H5	121.1
O1A—C1—O2A	125.2 (6)	C7—C6—H6	119.6
O1B—C1—O2B	121.6 (18)	C5—C6—H6	119.6
O2A—C1—C2	124.9 (5)	C6—C7—H7	119.3
O2B—C1—C2	120.2 (16)	C8—C7—H7	119.3

O1A—C1—C2	109.8 (5)	C9—C8—H8	121.1
O1B—C1—C2	117.8 (13)	C7—C8—H8	121.1
N1—C2—C1	110.5 (3)	N1—C10—H10A	111.4
N1—C2—C11	113.5 (3)	C9—C10—H10A	111.4
C1—C2—C11	113.4 (3)	N1—C10—H10B	111.4
O3—C3—N1	123.6 (3)	C9—C10—H10B	111.4
O3—C3—C4	129.4 (3)	H10A—C10—H10B	109.3
N1—C3—C4	107.0 (3)	C2—C11—H11A	108.4
C3—C4—C5	129.9 (3)	C12—C11—H11A	108.4
C3—C4—C9	108.4 (3)	C2—C11—H11B	108.4
C5—C4—C9	121.7 (3)	C12—C11—H11B	108.4
C4—C5—C6	117.7 (4)	H11A—C11—H11B	107.5
C5—C6—C7	120.8 (4)	C14—C12—H12	107.8
C6—C7—C8	121.5 (4)	C13—C12—H12	107.8
C7—C8—C9	117.8 (3)	C11—C12—H12	107.8
C4—C9—C8	120.5 (3)	C12—C13—H13A	109.5
C4—C9—C10	109.6 (3)	C12—C13—H13B	109.5
C8—C9—C10	129.9 (3)	H13A—C13—H13B	109.5
N1—C10—C9	101.7 (3)	C12—C13—H13C	109.5
C2—C11—C12	115.6 (3)	H13A—C13—H13C	109.5
C11—C12—C13	109.3 (3)	H13B—C13—H13C	109.5
C11—C12—C14	112.8 (3)	C12—C14—H14A	109.5
C13—C12—C14	111.0 (3)	C12—C14—H14B	109.5
C1—O1A—H1A	109.5	H14A—C14—H14B	109.5
C1—O1B—H2A	109.5	C12—C14—H14C	109.5
N1—C2—H2	106.3	H14A—C14—H14C	109.5
C11—C2—H2	106.3	H14B—C14—H14C	109.5

C3—N1—C2—C11	133.9 (3)	C9—C4—C5—C6	0.0 (5)
C3—N1—C2—C1	−97.4 (4)	C3—C4—C5—C6	179.5 (3)
O3—C3—N1—C2	−1.6 (5)	C4—C5—C6—C7	0.7 (5)
O1A—C1—C2—C11	−51.2 (9)	C5—C6—C7—C8	−0.3 (6)
C10—N1—C2—C11	−49.7 (4)	C6—C7—C8—C9	−0.8 (5)
C10—N1—C2—C1	79.0 (4)	C5—C4—C9—C8	−1.1 (5)
O2B—C1—C2—N1	−26 (3)	C3—C4—C9—C8	179.3 (3)
O2A—C1—C2—N1	4.0 (14)	C5—C4—C9—C10	178.5 (3)
O1B—C1—C2—N1	161 (3)	C3—C4—C9—C10	−1.1 (4)
O1A—C1—C2—N1	−179.9 (8)	C7—C8—C9—C4	1.4 (5)
O2B—C1—C2—C11	102 (3)	C7—C8—C9—C10	−178.0 (3)
O2A—C1—C2—C11	132.8 (13)	C3—N1—C10—C9	−1.7 (3)
O1B—C1—C2—C11	−71 (3)	C2—N1—C10—C9	−178.3 (3)
C10—N1—C3—O3	−178.3 (3)	C4—C9—C10—N1	1.6 (3)
C2—N1—C3—C4	177.8 (3)	C8—C9—C10—N1	−178.9 (3)
C10—N1—C3—C4	1.1 (3)	N1—C2—C11—C12	−55.7 (4)
O3—C3—C4—C9	179.4 (3)	C1—C2—C11—C12	177.2 (3)
N1—C3—C4—C9	0.0 (3)	C2—C11—C12—C14	−52.5 (4)
O3—C3—C4—C5	−0.2 (6)	C2—C11—C12—C13	−176.5 (3)
N1—C3—C4—C5	−179.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*A*···O3^{i}	0.82	1.83	2.634 (9)	168
C10—H10*A*···O3^{ii}	0.97	2.54	3.366 (4)	144
C8—H8···*Cg*1^{iii}	0.93	2.74	3.473 (4)	137
C2—H2···O3	0.98	2.38	2.812 (4)	106

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