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rac-Ethyl *rel*-(2*R*,3*R*,4*S*)-4-hydroxy-1,2-dimethyl-5-oxopyrrolidine-3-carboxylate

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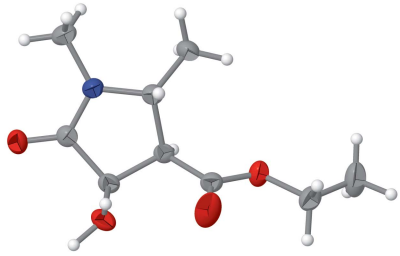
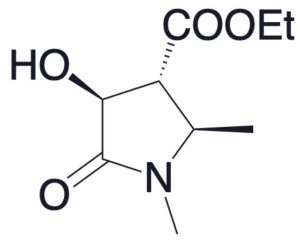
The asymmetric unit of the title compound, $C_9H_{15}NO_4$, consists of a functionalized pyrrolidine ring having an envelope conformation, synthesized as an ethyl ester. The molecule has three chiral centres and crystallized as a racemic mixture. In the crystal, molecules are linked by pairwise O—H···O bonds, generating dimers with twofold rotational symmetry.

3D view



Chemical scheme



Structure description

The heterocyclic compound 2-oxopyrrolidine and its derivatives have generated a lot of interest because of their practical significance (Pandya & Desai, 2020). These compounds have shown to be effective analgesics, anti-inflammatory (Salgın-Gökşen *et al.*, 2007), antiviral (Tian *et al.*, 2009), antimicrobial (Özkay *et al.*, 2010; Salgın-Gökşen *et al.*, 2007), antitumor (Abdel-Aziz *et al.*, 2021), anticonvulsant (Angelova *et al.*, 2016), anti-depressant (Kulandasamy *et al.*, 2009), cardioprotective (Ghazouani *et al.*, 2019) and antiplatelet agents (Mashayekhi *et al.*, 2013; Ghazouani *et al.*, 2019).

During the course of our study towards pyrrolidine-based iminosugars, we have synthesized the title compound by reduction of 2,3-dioxopyrrolidine (Bacho *et al.*, 2020; Abdul Rashid *et al.*, 2020). The starting material, 2,3-dioxopyrrolidine, was initially prepared *via* a multicomponent reaction, according to a previously reported procedure (Mohammat *et al.*, 2009, 2011).

The title compound crystallizes in the monoclinic crystal system, space group *C*2/*c*, with one molecule in the asymmetric unit (Fig. 1). The pyrrolidine ring (C1–C4/N1) adopts an envelope conformation, with atom C4 deviating by 0.180 (1) Å from the mean

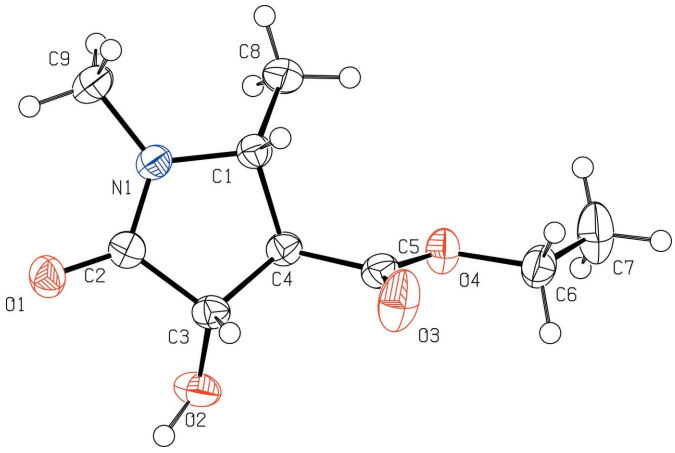


Figure 1
Crystal structure of the title compound, showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

plane. There are three chiral centres within the ring, at C4, with a C1—C4—C5—O4 torsion angle of −94.04 (11)°. The methyl and hydroxyl groups, attached to C1 and C3, respectively, are orientated awayfrom the mean plane with C2—N1—C1—C8 and N1—C2—C3—O2 torsion angles of 142.07 (10) and −135.48 (10)°, respectively. Meanwhile, the

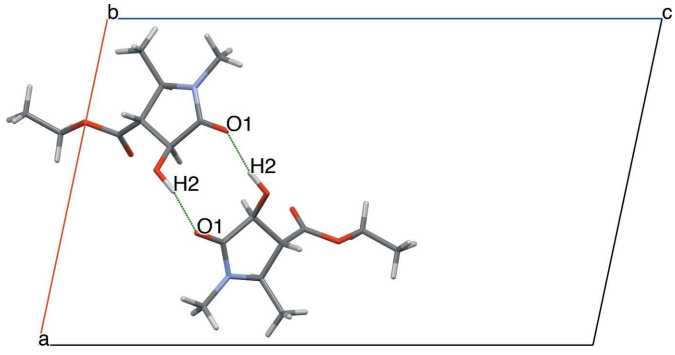


Figure 2
The O—H···O hydrogen bonds, indicated by green dashed bonds, forming $R_2^2(10)$ motifs in the crystal.

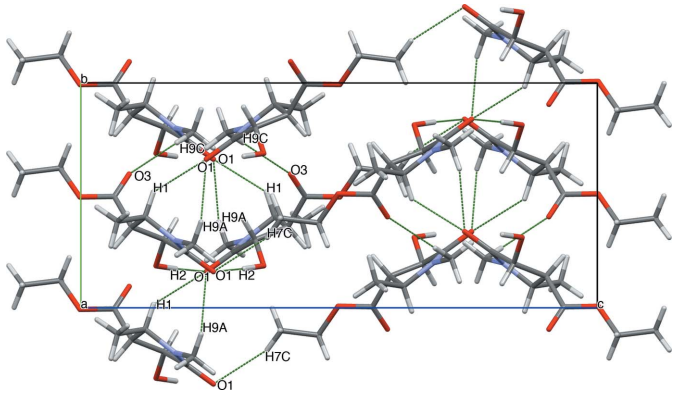


Figure 3
The molecular packing of title compound, viewed down the *a* axis. Intermolecular hydrogen bonds are indicated by green dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.97 (1)	1.78 (1)	2.7405 (12)	170 (2)
C1—H1···O1^{ii}	1.00	2.62	3.3953 (14)	134
C9—H9*A*···O1^{ii}	0.98	2.51	3.3355 (16)	142
C9—H9*C*···O3^{iii}	0.98	2.54	3.5086 (15)	169
C7—H7*C*···O1^{iv}	0.98	2.58	3.5134 (17)	160

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

ethyl ester group (O3/C5/O4/C6/C7) occupies the equatorial position on the pyrrolidine ring at C1, C3, and C4, . All bond lengths (Allen *et al.*, 1987) and angles in the molecule show normal values.

In the crystal, the molecules are linked by pairwise O—H···O hydrogen bonds, involving the carbonyl and hydroxy groups, forming centrosymmetric $R_2^2(10)$ ring motifs (Table 1, entry 1; Fig. 2). The packing also features C—H···O hydrogen bonds (Table 1), forming zigzag motifs propagating along the *c*-axis direction (Fig. 3).

Synthesis and crystallization

A solution of 2,3-dioxopyrrolidine (2.00 g, 10.04 mmol) together with Pd—C (10% wt; 1.39 g, 1.31 mmol) and acetic acid (4.59 ml, 80.32 mmol) was stirred in ethanol. The reaction was stirred vigorously under a hydrogen atmosphere to completion (24 h) and then filtered through Celite. After removal of the solvent, the crude product was purified by flash column chromatography on silica gel using ethyl acetate/petroleum ether (9/1), to afford two compounds; *trans*-hydroxyester **1** as a white solid and *cis*-hydroxyester **2** as a colourless oil. The white solid of *trans*-hydroxyester **1** was recrystallized from methanol solution to give single crystals of the title compound **1** (0.24 g, 12%).

trans-hydroxyester **1**: ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.57 (*d*, J = 8.5 Hz, 1H), 4.22 (*q*, J = 6.9 Hz, 2H), 3.63 (*s*, 1H), 2.82 (*s*, 3H), 2.67 (*t*, J = 8.4 Hz, 1H), 1.37 (*d*, J = 3.7 Hz, 3H), 1.29 (*t*, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 173.00 (C═O), 171.54 (C═O), 72.26 (CHOH), 61.71 (OCH_2), 54.35 (CH), 31.23 ($CHCH_3$), 27.33 (CH_3N), 19.31 (CH_3), 14.27 (CH_3); GCMS *m*/*z* (EI, +ve): found: 201.10 ([*M*]$^+$), calculated for $C_9H_{15}NO_4$: 201.10.

cis-hydroxyester **2**: (0.50 g, 25%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.44 (*d*, J = 7.3 Hz, 1H), 4.19 (*td*, J = 7.2, 4.9 Hz, 2H), 3.74 (*t*, J = 6.6 Hz, 1H), 3.38 (*t*, J = 6.6 Hz, 1H), 2.82 (*s*, 3H), 1.32–1.23 (*m*, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.82 (C═O), 169.59 (C═O), 70.88 (CHOH), 61.11 (OCH_2), 53.06 (CH), 49.21 ($CHCH_3$), 27.13 (CH_3N), 15.28 (CH_3), 14.37 (CH_3); GCMS *m*/*z* (EI, +ve): found: 201.10 ([*M*]$^+$), calculated for $C_9H_{15}NO_4$: 201.10.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_9H_{15}NO_4$
M_r	201.22
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	173
a, *b*, *c* (Å)	12.1599 (15), 8.6065 (8), 20.217 (2)
β (°)	101.960 (3)
V (Å^3)	2069.9 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.2 × 0.2 × 0.1
Data collection	
Diffractometer	Rigaku XtaLAB P200
Absorption correction	Multi-scan (*REQAB*; Rigaku, 1998)
T_{min}, T_{max}	0.879, 0.990
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11140, 1874, 1769
R_{int}	0.019
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.088, 1.04
No. of reflections	1874
No. of parameters	134
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.18

Computer programs: *CrystalClear-SM Expert* (Rigaku, 2015), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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full crystallographic data

IUCrData (2023). **8**, x230075 [https://doi.org/10.1107/S2414314623000755]

rac-Ethyl *rel*-(2*R*,3*R*,4*S*)-4-hydroxy-1,2-dimethyl-5-oxopyrrolidine-3-carboxylate

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Crystal data

$C_9H_{15}NO_4$
M_r = 201.22
Monoclinic, *C*2/*c*
a = 12.1599 (15) Å
b = 8.6065 (8) Å
c = 20.217 (2) Å
β = 101.960 (3)°
V = 2069.9 (4) Å^3
Z = 8
F(000) = 864
D_x = 1.291 Mg m^{-3}
Mo *K*α radiation, λ = 0.71075 Å
Cell parameters from 3484 reflections
θ = 2.1–27.5°
μ = 0.10 mm^{-1}
T = 173 K
Prism, colorless
0.2 × 0.2 × 0.1 mm

Data collection

Rigaku XtaLAB P200 diffractometer
Detector resolution: 5.814 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
T_{min} = 0.879, T_{max} = 0.990
11140 measured reflections
1874 independent reflections
1769 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 25.4°, θ_{min} = 2.1°
h = −14→14
k = −10→10
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.088
S = 1.04
1874 reflections
134 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2 + 1.1669P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Special details

Refinement. The hydroxyl H atom (H2) was refined with free coordinates and isotropic displacement parameter.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.65691 (7)	0.16087 (10)	0.24315 (4)	0.0360 (2)
O2	0.53577 (7)	0.18679 (11)	0.35435 (4)	0.0388 (2)
O3	0.58426 (9)	0.59491 (13)	0.40623 (5)	0.0556 (3)
O4	0.68278 (7)	0.49308 (10)	0.50163 (4)	0.0348 (2)
N1	0.78865 (8)	0.29976 (11)	0.31723 (5)	0.0282 (2)
C2	0.68560 (9)	0.24451 (13)	0.29333 (5)	0.0275 (3)
C3	0.60731 (9)	0.30292 (13)	0.33799 (5)	0.0278 (3)
H3	0.561557	0.391982	0.315420	0.033*
C4	0.68834 (9)	0.35965 (13)	0.40091 (5)	0.0259 (3)
H4	0.706096	0.271938	0.433837	0.031*
C1	0.79582 (9)	0.40440 (13)	0.37550 (5)	0.0275 (3)
H1	0.789576	0.514521	0.359380	0.033*
C9	0.88156 (10)	0.28015 (15)	0.28261 (6)	0.0359 (3)
H9A	0.902826	0.381524	0.267070	0.043*
H9B	0.858357	0.211119	0.243670	0.043*
H9C	0.946000	0.234634	0.313807	0.043*
C5	0.64421 (9)	0.49526 (13)	0.43501 (6)	0.0294 (3)
C6	0.64892 (11)	0.62159 (15)	0.54030 (6)	0.0364 (3)
H6A	0.566573	0.619870	0.537083	0.044*
H6B	0.669524	0.722225	0.522480	0.044*
C7	0.70872 (15)	0.60126 (19)	0.61170 (7)	0.0567 (4)
H7A	0.790035	0.600863	0.614059	0.068*
H7B	0.686220	0.502495	0.629065	0.068*
H7C	0.689349	0.687011	0.639073	0.068*
C8	0.90310 (10)	0.38489 (16)	0.42851 (6)	0.0374 (3)
H8A	0.967321	0.419643	0.410005	0.045*
H8B	0.912839	0.275194	0.441383	0.045*
H8C	0.898462	0.447241	0.468402	0.045*
H2	0.4729 (10)	0.174 (2)	0.3162 (6)	0.063 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0353 (5)	0.0407 (5)	0.0292 (4)	0.0041 (4)	0.0005 (3)	−0.0061 (4)
O2	0.0307 (4)	0.0512 (5)	0.0333 (5)	−0.0129 (4)	0.0038 (4)	0.0043 (4)
O3	0.0666 (7)	0.0579 (7)	0.0377 (5)	0.0363 (5)	0.0007 (5)	−0.0005 (4)
O4	0.0418 (5)	0.0345 (5)	0.0271 (4)	0.0084 (4)	0.0048 (3)	−0.0033 (3)
N1	0.0256 (5)	0.0321 (5)	0.0274 (5)	0.0024 (4)	0.0067 (4)	0.0004 (4)
C2	0.0280 (5)	0.0283 (6)	0.0247 (5)	0.0033 (4)	0.0022 (4)	0.0041 (4)
C3	0.0239 (5)	0.0324 (6)	0.0262 (6)	0.0001 (4)	0.0031 (4)	0.0030 (4)
C4	0.0238 (5)	0.0286 (6)	0.0247 (5)	0.0024 (4)	0.0034 (4)	0.0025 (4)
C1	0.0257 (5)	0.0273 (5)	0.0296 (6)	0.0003 (4)	0.0061 (4)	−0.0003 (4)
C9	0.0297 (6)	0.0449 (7)	0.0353 (6)	0.0061 (5)	0.0118 (5)	0.0014 (5)
C5	0.0248 (5)	0.0342 (6)	0.0291 (6)	0.0029 (5)	0.0054 (4)	0.0014 (5)
C6	0.0399 (7)	0.0341 (6)	0.0370 (7)	0.0036 (5)	0.0126 (5)	−0.0060 (5)

C7	0.0757 (10)	0.0528 (9)	0.0374 (7)	0.0168 (8)	0.0023 (7)	−0.0136 (6)
C8	0.0252 (6)	0.0478 (7)	0.0372 (6)	−0.0010 (5)	0.0021 (5)	−0.0065 (5)

Geometric parameters (Å, º)

O1—C2	1.2340 (14)	C1—H1	1.0000
O2—C3	1.4087 (14)	C1—C8	1.5162 (16)
O2—H2	0.973 (5)	C9—H9A	0.9800
O3—C5	1.1957 (14)	C9—H9B	0.9800
O4—C5	1.3313 (14)	C9—H9C	0.9800
O4—C6	1.4620 (14)	C6—H6A	0.9900
N1—C2	1.3337 (15)	C6—H6B	0.9900
N1—C1	1.4709 (14)	C6—C7	1.4860 (19)
N1—C9	1.4569 (14)	C7—H7A	0.9800
C2—C3	1.5266 (15)	C7—H7B	0.9800
C3—H3	1.0000	C7—H7C	0.9800
C3—C4	1.5192 (15)	C8—H8A	0.9800
C4—H4	1.0000	C8—H8B	0.9800
C4—C1	1.5488 (14)	C8—H8C	0.9800
C4—C5	1.5095 (15)		
C3—O2—H2	108.5 (10)	N1—C9—H9B	109.5
C5—O4—C6	116.81 (9)	N1—C9—H9C	109.5
C2—N1—C1	113.81 (9)	H9A—C9—H9B	109.5
C2—N1—C9	123.27 (10)	H9A—C9—H9C	109.5
C9—N1—C1	122.17 (9)	H9B—C9—H9C	109.5
O1—C2—N1	126.17 (10)	O3—C5—O4	123.63 (11)
O1—C2—C3	125.01 (10)	O3—C5—C4	124.81 (10)
N1—C2—C3	108.82 (9)	O4—C5—C4	111.53 (9)
O2—C3—C2	113.35 (10)	O4—C6—H6A	110.3
O2—C3—H3	109.8	O4—C6—H6B	110.3
O2—C3—C4	110.88 (9)	O4—C6—C7	107.16 (10)
C2—C3—H3	109.8	H6A—C6—H6B	108.5
C4—C3—C2	103.02 (8)	C7—C6—H6A	110.3
C4—C3—H3	109.8	C7—C6—H6B	110.3
C3—C4—H4	109.1	C6—C7—H7A	109.5
C3—C4—C1	104.33 (8)	C6—C7—H7B	109.5
C1—C4—H4	109.1	C6—C7—H7C	109.5
C5—C4—C3	113.62 (9)	H7A—C7—H7B	109.5
C5—C4—H4	109.1	H7A—C7—H7C	109.5
C5—C4—C1	111.32 (9)	H7B—C7—H7C	109.5
N1—C1—C4	101.50 (8)	C1—C8—H8A	109.5
N1—C1—H1	109.4	C1—C8—H8B	109.5
N1—C1—C8	113.44 (9)	C1—C8—H8C	109.5
C4—C1—H1	109.4	H8A—C8—H8B	109.5
C8—C1—C4	113.55 (9)	H8A—C8—H8C	109.5
C8—C1—H1	109.4	H8B—C8—H8C	109.5
N1—C9—H9A	109.5		

O1—C2—C3—O2	45.04 (15)	C1—N1—C2—O1	176.42 (11)
O1—C2—C3—C4	164.92 (11)	C1—N1—C2—C3	−3.06 (12)
O2—C3—C4—C1	148.36 (9)	C1—C4—C5—O3	84.29 (14)
O2—C3—C4—C5	−90.22 (11)	C1—C4—C5—O4	−94.04 (11)
N1—C2—C3—O2	−135.48 (10)	C9—N1—C2—O1	6.15 (18)
N1—C2—C3—C4	−15.60 (12)	C9—N1—C2—C3	−173.33 (10)
C2—N1—C1—C4	19.89 (12)	C9—N1—C1—C4	−169.72 (9)
C2—N1—C1—C8	142.07 (10)	C9—N1—C1—C8	−47.54 (14)
C2—C3—C4—C1	26.79 (11)	C5—O4—C6—C7	−175.57 (11)
C2—C3—C4—C5	148.21 (9)	C5—C4—C1—N1	−151.06 (9)
C3—C4—C1—N1	−28.13 (10)	C5—C4—C1—C8	86.83 (11)
C3—C4—C1—C8	−150.24 (10)	C6—O4—C5—O3	−0.29 (17)
C3—C4—C5—O3	−33.14 (16)	C6—O4—C5—C4	178.06 (9)
C3—C4—C5—O4	148.53 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.97 (1)	1.78 (1)	2.7405 (12)	170 (2)
C1—H1···O1^{ii}	1.00	2.62	3.3953 (14)	134
C9—H9*A*···O1^{ii}	0.98	2.51	3.3355 (16)	142
C9—H9*C*···O3^{iii}	0.98	2.54	3.5086 (15)	169
C7—H7*C*···O1^{iv}	0.98	2.58	3.5134 (17)	160

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