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(–)-(4*R*,5*S*)-4-Methyl-3-[2(*S*)-phenoxypropionyl]-5-phenyloxazolidin-2-one

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Key indicators

Single-crystal X-ray study
T = 160 K
Mean σ(C–C) = 0.004 Å
R factor = 0.029
wR factor = 0.067
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.

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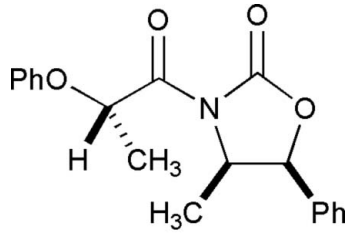
The title compound, $C_{19}H_{19}NO_4$, formed from enantiomerically pure (+)-(4*R*,5S)-4-methyl-5-phenyl-2-oxazolidinone and racemic 2-phenoxypropanoyl chloride, crystallises with $Z' = 2$. The two carbonyl groups in each molecule are oriented *anti* to each other, while the two methyl groups are oriented *syn* to each other.

Comment

The title compound, (I), is the sixth in a series of structurally related compounds, introduced in our earlier report (Coumbarides, Eames *et al.*, 2006*a*). With $R^1 = C_6H_5O$, the reaction shown in that report yielded the *anti–syn* and *syn–syn* diastereomers in 44 and 45% yields, respectively. The *syn–syn* diastereomer was described previously (Coumbarides, Eames *et al.*, 2006*b*). The title compound, (I), is the *anti–syn* diastereomer.



(I)

Compound (I) contains two molecules in the asymmetric unit in the space group $P2_1$, displaying closely comparable conformations (Fig. 1). In line with our previous reports (Coumbarides, Eames *et al.*, 2006*a*,*b*; Coumbarides, Dingjan *et al.*, 2006; Chavda *et al.*, 2006*a*,*b*), the carbonyl groups (C3*A*═O2*A*/C11*A*═O3*A* and C3*B*═O2*B*/C11*B*═O3*B*) are oriented *anti* to each other, with torsion angles O3—C11—N1—C3 = 176.5 (2) and 175.9 (2)° for molecules *A* and *B*, respectively. The two methyl groups (C4*A*/C19*A* and C4*B*/C19*B*) lie to the same side of the molecule. The principal distinction between the two independent molecules of (I) lies in the orientations of the phenoxypropionyl substituent with respect to the central portion of the molecule, with torsion angles O3—C11—C12—O4 = −25.6 (3) and −14.6 (3)° for molecules *A* and *B*, respectively. This subtle difference can be attributed to the influence of intermolecular interactions in the solid state. As observed in the phenylpropionyl derivative (Coumbarides, Eames *et al.*, 2006*a*), adjacent molecules approach each other in a 'side-on' manner (Fig. 2), and the shortest intermolecular contacts are C—H···O interactions (Table 1).

Experimental

The title compound was obtained from the same synthesis as the *syn–syn* diastereomer, as reported previously (Coumbarides, Eames *et al.*, 2006*b*). The *anti–syn* diastereomer, (I), was obtained as colourless crystals {4.03 g, 44% yield, m.p. 362–365 K, R_F 0.61 [light petroleum (b.p 313–333 K)/diethyl ether, 1:1]}. Spectroscopic analysis: $[\alpha]_D^{22}$ = −35.5 ($CHCl_3$, 293 K, concentration 2.0 g per 100 ml); IR ($CHCl_3$, ν_{max}, cm^{-1}): 1776 (C═O), 1714 (C═O); ^1H NMR (270 MHz, $CDCl_3$): δ 7.45–7.21 (7H, *m*, 7 × CH; Ph_a and Ph_b), 6.97–6.86 (3H, *m*, 3 × CH; Ph_a or Ph_b), 5.94 (1H, *q*, *J* = 6.7 Hz, PhOCH), 5.75 (1H, *d*, *J* = 7.4 Hz, PhCHO), 4.81 (1H, *m*, CHN), 1.66 (3H, *d*, *J* = 6.7 Hz, CH_3CHCO), 0.89 (3H, *d*, *J* = 6.6 Hz, CH_3CHN); ^{13}C NMR (67.9 MHz, $CDCl_3$, δ, p.p.m.): 172.0 (NC=O), 157.4 (*i*-CO; Ph), 152.8 (OC═O), 133.1 (*i*-C; Ph), 129.7, 129.0, 128.9, 125.7, 121.6, 115.1 (6 × CH; Ph_a and Ph_b), 79.8 (PhCHO), 71.8 (PhOCH), 54.7 (CHN), 18.3 (CH_3), 14.5 (CH_3); found: MH^+ 326.1393; $C_{19}H_{20}NO_4$ requires 326.1392.

Crystal data

$C_{19}H_{19}NO_4$
M_r = 325.35
Monoclinic, $P2_1$
a = 11.268 (7) Å
b = 10.493 (5) Å
c = 15.008 (9) Å
β = 102.96 (4)°
V = 1729.3 (17) Å^3
Z = 4
D_x = 1.250 Mg m^{-3}
Mo *K*α radiation
μ = 0.09 mm^{-1}
T = 160 (2) K
Block, colourless
0.44 × 0.22 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
8490 measured reflections
3223 independent reflections
2662 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.0°
2 standard reflections
every 100 reflections
intensity decay: 2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.067
S = 1.01
3223 reflections
438 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 0.3025P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0167 (13)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1*A*—H1*A*···O3*B*	1.00	2.61	3.373 (3)	133
C1*B*—H1*B*···O3*A*	1.00	2.57	3.568 (3)	174
C18*A*—H18*A*···O4*B*^{i}	0.95	2.52	3.445 (4)	165
C18*B*—H18*B*···O4*A*^{ii}	0.95	2.69	3.564 (4)	154

Symmetry codes: (i) $x+1, y, z$; (ii) $x-1, y, z$.

H atoms were placed in geometrically idealised positions and constrained to ride on their parent atoms, with C—H = 0.95–1.00 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate about their local threefold axes. In the absence of significant anomalous scattering effects, the few measured Friedel pairs have been merged. The absolute configuration is assigned on the basis of the known configuration of the starting material (Coumbarides, Eames *et al.*, 2006*a*).

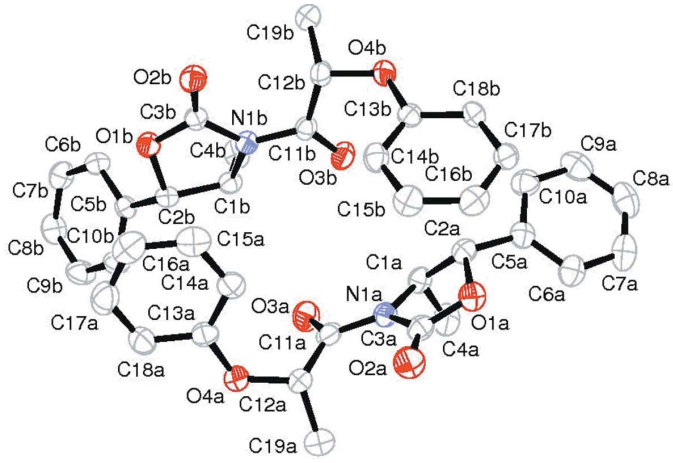


Figure 1
Two molecules in the asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted.

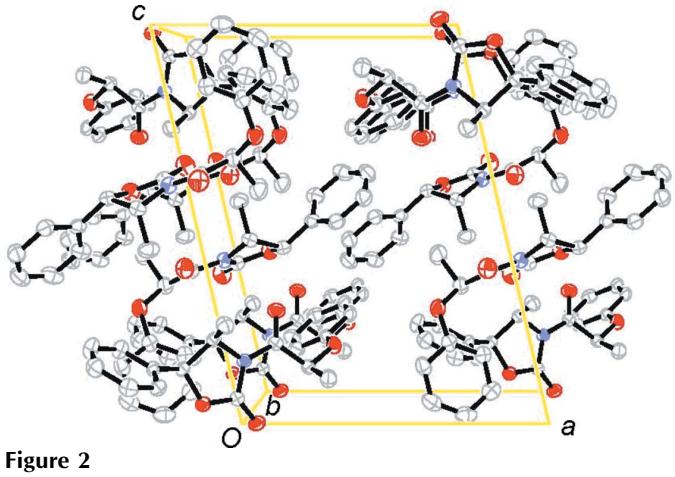


Figure 2
The crystal packing of (I) viewed along the *b* axis. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted.

Data collection: *CAD-4-PC* Software (Enraf–Nonius, 1994); cell refinement: *CAD-4-PC* Software; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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supporting information

Acta Cryst. (2006). E**62**, o4043–o4045 [https://doi.org/10.1107/S1600536806031850]

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Crystal data

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Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 11.268$ (7) Å
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$c = 15.008$ (9) Å
$\beta = 102.96$ (4)°
$V = 1729.3$ (17) Å^3
$Z = 4$
$F(000) = 688$
$D_x = 1.250$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 9.3$–$12.1°$
$\mu = 0.09$ mm^{-1}
$T = 160$ K
Block, colourless
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Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
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$\omega/2\theta$ scans
8490 measured reflections
3223 independent reflections
2662 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -13 \rightarrow 13$
$k = -12 \rightarrow 10$
$l = -17 \rightarrow 17$
2 standard reflections every 100 reflections
intensity decay: 2%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.067$
$S = 1.01$
3223 reflections
438 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 0.3025P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0167 (13)
Absolute structure: assigned on the basis of known starting material

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 $F^2 > 2\sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1A	0.8590 (2)	0.7252 (2)	0.54614 (16)	0.0319 (6)
H1A	0.8515	0.6363	0.5682	0.038*
C2A	0.7607 (2)	0.8113 (2)	0.56925 (17)	0.0316 (6)
H2A	0.7433	0.7824	0.6285	0.038*
C3A	0.9406 (2)	0.9171 (3)	0.61434 (17)	0.0331 (6)
C4A	0.8647 (3)	0.7257 (3)	0.44639 (17)	0.0457 (7)
H4A	0.7937	0.6806	0.4104	0.069*
H4B	0.9393	0.6828	0.4393	0.069*
H4C	0.8647	0.8138	0.4248	0.069*
C5A	0.6427 (2)	0.8218 (3)	0.49987 (17)	0.0335 (6)
C6A	0.6187 (3)	0.9201 (3)	0.43665 (18)	0.0418 (7)
H6A	0.6786	0.9833	0.4352	0.050*
C7A	0.5059 (3)	0.9253 (3)	0.37521 (19)	0.0495 (8)
H7A	0.4884	0.9933	0.3325	0.059*
C8A	0.4199 (3)	0.8328 (3)	0.3761 (2)	0.0513 (8)
H8A	0.3428	0.8379	0.3346	0.062*
C9A	0.4449 (3)	0.7325 (3)	0.4367 (2)	0.0499 (8)
H9A	0.3862	0.6672	0.4357	0.060*
C10A	0.5557 (2)	0.7274 (3)	0.49909 (17)	0.0417 (7)
H10A	0.5725	0.6591	0.5416	0.050*
C11A	1.0786 (2)	0.7267 (3)	0.62787 (17)	0.0350 (6)
C12A	1.1896 (2)	0.8077 (3)	0.66833 (18)	0.0385 (7)
H12A	1.1671	0.8796	0.7050	0.046*
C13A	1.2699 (2)	0.7019 (2)	0.81044 (18)	0.0356 (6)
C14A	1.1665 (2)	0.7249 (3)	0.84300 (18)	0.0357 (6)
H14A	1.0964	0.7617	0.8044	0.043*
C15A	1.1664 (3)	0.6934 (3)	0.93299 (19)	0.0419 (7)
H15A	1.0958	0.7094	0.9560	0.050*
C16A	1.2674 (3)	0.6392 (3)	0.98927 (19)	0.0481 (8)
H16A	1.2665	0.6174	1.0506	0.058*
C17A	1.3694 (3)	0.6170 (3)	0.9555 (2)	0.0509 (8)
H17A	1.4393	0.5800	0.9941	0.061*
C18A	1.3717 (2)	0.6475 (3)	0.8669 (2)	0.0438 (7)
H18A	1.4427	0.6313	0.8444	0.053*
C19A	1.2426 (3)	0.8579 (4)	0.5903 (2)	0.0593 (9)

H19A	1.3156	0.9084	0.6153	0.089*
H19B	1.1821	0.9114	0.5501	0.089*
H19C	1.2642	0.7860	0.5553	0.089*
N1A	0.96725 (18)	0.78883 (19)	0.60150 (13)	0.0305 (5)
O1A	0.82054 (15)	0.93517 (17)	0.58309 (11)	0.0348 (4)
O2A	1.00899 (18)	1.00028 (19)	0.64643 (14)	0.0451 (5)
O3A	1.08465 (17)	0.61293 (19)	0.61517 (14)	0.0444 (5)
O4A	1.28192 (15)	0.73015 (19)	0.72346 (13)	0.0426 (5)
C1B	1.0157 (2)	0.3999 (2)	0.78187 (16)	0.0285 (5)
H1B	1.0282	0.4597	0.7329	0.034*
C2B	1.1357 (2)	0.3824 (2)	0.85379 (16)	0.0271 (5)
H2B	1.1861	0.4611	0.8547	0.033*
C3B	0.9894 (2)	0.4373 (2)	0.93148 (16)	0.0272 (5)
C4B	0.9561 (2)	0.2784 (3)	0.73972 (18)	0.0382 (6)
H4D	0.9424	0.2214	0.7882	0.057*
H4E	1.0094	0.2363	0.7053	0.057*
H4F	0.8780	0.2987	0.6984	0.057*
C5B	1.2131 (2)	0.2691 (2)	0.84494 (16)	0.0268 (5)
C6B	1.1944 (2)	0.1511 (2)	0.88184 (17)	0.0323 (6)
H6B	1.1307	0.1404	0.9133	0.039*
C7B	1.2689 (2)	0.0491 (3)	0.87271 (18)	0.0389 (6)
H7B	1.2567	−0.0310	0.8987	0.047*
C8B	1.3605 (3)	0.0633 (3)	0.82617 (19)	0.0416 (7)
H8B	1.4109	−0.0072	0.8197	0.050*
C9B	1.3792 (3)	0.1801 (3)	0.7888 (2)	0.0444 (7)
H9B	1.4420	0.1900	0.7564	0.053*
C10B	1.3060 (2)	0.2825 (3)	0.79896 (18)	0.0364 (6)
H10B	1.3196	0.3630	0.7740	0.044*
C11B	0.8321 (2)	0.5233 (2)	0.79965 (16)	0.0274 (5)
C12B	0.7449 (2)	0.5565 (3)	0.86101 (17)	0.0311 (6)
H12B	0.7897	0.5979	0.9188	0.037*
C13B	0.6818 (2)	0.7632 (2)	0.79734 (16)	0.0285 (6)
C14B	0.7941 (2)	0.8189 (3)	0.83231 (17)	0.0354 (6)
H14B	0.8579	0.7710	0.8696	0.043*
C15B	0.8120 (2)	0.9456 (3)	0.81206 (18)	0.0401 (7)
H15B	0.8887	0.9846	0.8358	0.048*
C16B	0.7199 (2)	1.0154 (3)	0.75805 (17)	0.0393 (7)
H16B	0.7330	1.1019	0.7443	0.047*
C17B	0.6082 (2)	0.9585 (3)	0.72391 (18)	0.0365 (6)
H17B	0.5444	1.0066	0.6868	0.044*
C18B	0.5883 (2)	0.8326 (3)	0.74319 (17)	0.0339 (6)
H18B	0.5114	0.7941	0.7196	0.041*
C19B	0.6798 (2)	0.4372 (3)	0.88171 (19)	0.0416 (7)
H19D	0.6253	0.4589	0.9219	0.062*
H19E	0.7399	0.3745	0.9120	0.062*
H19F	0.6322	0.4012	0.8245	0.062*
N1B	0.94126 (17)	0.46148 (19)	0.83903 (12)	0.0266 (5)
O1B	1.09520 (14)	0.37535 (16)	0.93983 (10)	0.0299 (4)

O2B	0.94664 (15)	0.46410 (18)	0.99534 (11)	0.0359 (4)
O3B	0.80738 (16)	0.54245 (18)	0.71840 (11)	0.0367 (4)
O4B	0.65259 (14)	0.63842 (17)	0.81217 (12)	0.0336 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.0374 (13)	0.0248 (14)	0.0319 (13)	0.0009 (11)	0.0041 (11)	−0.0011 (11)
C2A	0.0384 (14)	0.0294 (15)	0.0275 (13)	0.0002 (12)	0.0083 (10)	−0.0005 (11)
C3A	0.0399 (15)	0.0279 (15)	0.0323 (13)	0.0002 (13)	0.0101 (12)	0.0003 (11)
C4A	0.0543 (17)	0.0488 (19)	0.0348 (15)	0.0156 (15)	0.0118 (13)	−0.0043 (14)
C5A	0.0371 (14)	0.0350 (15)	0.0296 (13)	0.0077 (12)	0.0102 (11)	−0.0040 (11)
C6A	0.0489 (16)	0.0362 (17)	0.0392 (15)	0.0063 (14)	0.0074 (13)	−0.0031 (13)
C7A	0.0586 (18)	0.0431 (18)	0.0402 (16)	0.0163 (16)	−0.0027 (13)	−0.0040 (14)
C8A	0.0396 (16)	0.063 (2)	0.0456 (17)	0.0103 (16)	−0.0024 (13)	−0.0122 (16)
C9A	0.0392 (16)	0.062 (2)	0.0486 (17)	−0.0055 (15)	0.0110 (14)	−0.0136 (17)
C10A	0.0449 (16)	0.0462 (18)	0.0354 (14)	−0.0016 (14)	0.0120 (12)	−0.0003 (13)
C11A	0.0405 (15)	0.0345 (18)	0.0332 (14)	0.0039 (13)	0.0154 (11)	0.0094 (12)
C12A	0.0340 (14)	0.0377 (17)	0.0433 (15)	0.0011 (12)	0.0080 (12)	0.0137 (13)
C13A	0.0354 (14)	0.0266 (15)	0.0443 (16)	−0.0061 (12)	0.0077 (12)	0.0028 (12)
C14A	0.0368 (15)	0.0269 (14)	0.0431 (15)	−0.0036 (12)	0.0086 (12)	−0.0018 (12)
C15A	0.0534 (17)	0.0281 (16)	0.0466 (17)	−0.0082 (13)	0.0164 (14)	−0.0132 (13)
C16A	0.066 (2)	0.0400 (19)	0.0352 (15)	−0.0138 (16)	0.0052 (14)	−0.0049 (13)
C17A	0.0505 (18)	0.048 (2)	0.0459 (18)	−0.0082 (16)	−0.0063 (14)	0.0062 (15)
C18A	0.0317 (14)	0.0439 (18)	0.0532 (18)	−0.0043 (13)	0.0037 (13)	0.0060 (14)
C19A	0.0462 (18)	0.070 (2)	0.063 (2)	−0.0015 (16)	0.0161 (16)	0.0254 (18)
N1A	0.0323 (11)	0.0244 (12)	0.0354 (11)	0.0024 (9)	0.0086 (9)	0.0018 (9)
O1A	0.0389 (10)	0.0283 (10)	0.0368 (10)	0.0029 (8)	0.0075 (8)	−0.0058 (8)
O2A	0.0461 (11)	0.0287 (11)	0.0581 (12)	−0.0046 (9)	0.0067 (9)	−0.0042 (9)
O3A	0.0464 (11)	0.0314 (12)	0.0556 (12)	0.0092 (9)	0.0119 (9)	0.0022 (9)
O4A	0.0321 (9)	0.0500 (13)	0.0469 (11)	0.0053 (9)	0.0113 (8)	0.0172 (9)
C1B	0.0321 (13)	0.0260 (14)	0.0297 (12)	0.0025 (11)	0.0119 (10)	0.0006 (10)
C2B	0.0289 (13)	0.0255 (14)	0.0286 (12)	−0.0026 (10)	0.0102 (10)	−0.0006 (10)
C3B	0.0282 (12)	0.0232 (13)	0.0298 (13)	−0.0006 (11)	0.0058 (10)	0.0000 (10)
C4B	0.0368 (14)	0.0369 (16)	0.0386 (14)	0.0012 (12)	0.0035 (11)	−0.0094 (12)
C5B	0.0251 (12)	0.0261 (14)	0.0290 (12)	0.0016 (10)	0.0052 (10)	−0.0021 (10)
C6B	0.0354 (14)	0.0296 (15)	0.0335 (14)	−0.0027 (12)	0.0111 (11)	0.0003 (11)
C7B	0.0486 (16)	0.0257 (15)	0.0407 (15)	0.0041 (13)	0.0065 (12)	0.0004 (12)
C8B	0.0420 (15)	0.0344 (17)	0.0476 (16)	0.0128 (13)	0.0085 (13)	−0.0068 (13)
C9B	0.0395 (16)	0.0451 (19)	0.0546 (17)	0.0038 (13)	0.0231 (13)	−0.0010 (14)
C10B	0.0377 (15)	0.0302 (15)	0.0447 (15)	0.0004 (12)	0.0165 (12)	0.0011 (12)
C11B	0.0294 (13)	0.0229 (14)	0.0286 (13)	−0.0008 (10)	0.0036 (10)	0.0016 (10)
C12B	0.0302 (13)	0.0310 (15)	0.0314 (13)	0.0073 (11)	0.0058 (10)	0.0050 (11)
C13B	0.0302 (13)	0.0290 (15)	0.0288 (12)	0.0045 (11)	0.0121 (10)	−0.0001 (11)
C14B	0.0357 (14)	0.0390 (17)	0.0295 (13)	0.0041 (13)	0.0029 (11)	−0.0006 (12)
C15B	0.0423 (15)	0.0375 (17)	0.0388 (15)	−0.0037 (14)	0.0052 (12)	−0.0044 (13)
C16B	0.0507 (17)	0.0329 (16)	0.0368 (15)	0.0036 (13)	0.0148 (13)	−0.0011 (12)
C17B	0.0350 (14)	0.0352 (17)	0.0431 (15)	0.0122 (13)	0.0165 (11)	0.0092 (13)

C18B	0.0270 (13)	0.0380 (17)	0.0384 (14)	0.0086 (12)	0.0109 (11)	0.0053 (12)
C19B	0.0380 (15)	0.0421 (18)	0.0454 (16)	0.0046 (14)	0.0111 (12)	0.0152 (14)
N1B	0.0298 (10)	0.0259 (12)	0.0247 (10)	0.0025 (9)	0.0073 (8)	−0.0012 (8)
O1B	0.0310 (9)	0.0327 (10)	0.0268 (9)	0.0056 (8)	0.0083 (7)	−0.0004 (7)
O2B	0.0396 (10)	0.0432 (11)	0.0272 (9)	0.0085 (9)	0.0121 (8)	0.0003 (8)
O3B	0.0414 (10)	0.0384 (11)	0.0293 (10)	0.0078 (9)	0.0059 (8)	0.0060 (8)
O4B	0.0281 (9)	0.0305 (10)	0.0417 (10)	0.0045 (8)	0.0069 (8)	0.0081 (8)

Geometric parameters (Å, º)

C1A—N1A	1.472 (3)	C1B—N1B	1.476 (3)
C1A—C4A	1.513 (4)	C1B—C4B	1.512 (4)
C1A—C2A	1.528 (4)	C1B—C2B	1.540 (3)
C1A—H1A	1.000	C1B—H1B	1.000
C2A—O1A	1.457 (3)	C2B—O1B	1.465 (3)
C2A—C5A	1.498 (4)	C2B—C5B	1.498 (3)
C2A—H2A	1.000	C2B—H2B	1.0000
C3A—O2A	1.192 (3)	C3B—O2B	1.199 (3)
C3A—O1A	1.343 (3)	C3B—O1B	1.339 (3)
C3A—N1A	1.401 (4)	C3B—N1B	1.395 (3)
C4A—H4A	0.980	C4B—H4D	0.980
C4A—H4B	0.980	C4B—H4E	0.980
C4A—H4C	0.980	C4B—H4F	0.980
C5A—C6A	1.387 (4)	C5B—C10B	1.384 (4)
C5A—C10A	1.392 (4)	C5B—C6B	1.391 (4)
C6A—C7A	1.394 (4)	C6B—C7B	1.385 (4)
C6A—H6A	0.950	C6B—H6B	0.9500
C7A—C8A	1.374 (5)	C7B—C8B	1.378 (4)
C7A—H7A	0.950	C7B—H7B	0.950
C8A—C9A	1.378 (5)	C8B—C9B	1.384 (4)
C8A—H8A	0.950	C8B—H8B	0.950
C9A—C10A	1.384 (4)	C9B—C10B	1.383 (4)
C9A—H9A	0.950	C9B—H9B	0.950
C10A—H10A	0.950	C10B—H10B	0.950
C11A—O3A	1.213 (3)	C11B—O3B	1.205 (3)
C11A—N1A	1.390 (3)	C11B—N1B	1.399 (3)
C11A—C12A	1.522 (4)	C11B—C12B	1.529 (3)
C12A—O4A	1.429 (3)	C12B—O4B	1.420 (3)
C12A—C19A	1.522 (4)	C12B—C19B	1.518 (4)
C12A—H12A	1.000	C12B—H12B	1.000
C13A—O4A	1.375 (3)	C13B—O4B	1.380 (3)
C13A—C14A	1.382 (4)	C13B—C14B	1.386 (4)
C13A—C18A	1.387 (4)	C13B—C18B	1.384 (3)
C14A—C15A	1.391 (4)	C14B—C15B	1.389 (4)
C14A—H14A	0.950	C14B—H14B	0.950
C15A—C16A	1.379 (4)	C15B—C16B	1.375 (4)
C15A—H15A	0.950	C15B—H15B	0.950
C16A—C17A	1.376 (4)	C16B—C17B	1.384 (4)

C16A—H16A	0.950	C16B—H16B	0.950
C17A—C18A	1.374 (4)	C17B—C18B	1.381 (4)
C17A—H17A	0.950	C17B—H17B	0.950
C18A—H18A	0.950	C18B—H18B	0.950
C19A—H19A	0.980	C19B—H19D	0.980
C19A—H19B	0.980	C19B—H19E	0.980
C19A—H19C	0.980	C19B—H19F	0.980
N1A—C1A—C4A	110.1 (2)	N1B—C1B—C4B	110.8 (2)
N1A—C1A—C2A	98.90 (19)	N1B—C1B—C2B	99.74 (18)
C4A—C1A—C2A	114.6 (2)	C4B—C1B—C2B	115.5 (2)
N1A—C1A—H1A	110.9	N1B—C1B—H1B	110.1
C4A—C1A—H1A	110.9	C4B—C1B—H1B	110.1
C2A—C1A—H1A	110.9	C2B—C1B—H1B	110.1
O1A—C2A—C5A	110.1 (2)	O1B—C2B—C5B	109.91 (19)
O1A—C2A—C1A	102.94 (19)	O1B—C2B—C1B	103.03 (18)
C5A—C2A—C1A	117.5 (2)	C5B—C2B—C1B	118.0 (2)
O1A—C2A—H2A	108.7	O1B—C2B—H2B	108.5
C5A—C2A—H2A	108.7	C5B—C2B—H2B	108.5
C1A—C2A—H2A	108.7	C1B—C2B—H2B	108.5
O2A—C3A—O1A	123.2 (3)	O2B—C3B—O1B	123.2 (2)
O2A—C3A—N1A	128.3 (2)	O2B—C3B—N1B	128.0 (2)
O1A—C3A—N1A	108.5 (2)	O1B—C3B—N1B	108.71 (19)
C1A—C4A—H4A	109.5	C1B—C4B—H4D	109.5
C1A—C4A—H4B	109.5	C1B—C4B—H4E	109.5
H4A—C4A—H4B	109.5	H4D—C4B—H4E	109.5
C1A—C4A—H4C	109.5	C1B—C4B—H4F	109.5
H4A—C4A—H4C	109.5	H4D—C4B—H4F	109.5
H4B—C4A—H4C	109.5	H4E—C4B—H4F	109.5
C6A—C5A—C10A	119.7 (2)	C10B—C5B—C6B	119.2 (2)
C6A—C5A—C2A	122.4 (2)	C10B—C5B—C2B	118.9 (2)
C10A—C5A—C2A	117.9 (2)	C6B—C5B—C2B	121.9 (2)
C5A—C6A—C7A	119.4 (3)	C7B—C6B—C5B	119.9 (2)
C5A—C6A—H6A	120.3	C7B—C6B—H6B	120.0
C7A—C6A—H6A	120.3	C5B—C6B—H6B	120.0
C8A—C7A—C6A	120.4 (3)	C8B—C7B—C6B	120.4 (3)
C8A—C7A—H7A	119.8	C8B—C7B—H7B	119.8
C6A—C7A—H7A	119.8	C6B—C7B—H7B	119.8
C7A—C8A—C9A	120.4 (3)	C7B—C8B—C9B	120.0 (3)
C7A—C8A—H8A	119.8	C7B—C8B—H8B	120.0
C9A—C8A—H8A	119.8	C9B—C8B—H8B	120.0
C8A—C9A—C10A	119.7 (3)	C8B—C9B—C10B	119.6 (3)
C8A—C9A—H9A	120.1	C8B—C9B—H9B	120.2
C10A—C9A—H9A	120.1	C10B—C9B—H9B	120.2
C9A—C10A—C5A	120.3 (3)	C5B—C10B—C9B	120.8 (3)
C9A—C10A—H10A	119.8	C5B—C10B—H10B	119.6
C5A—C10A—H10A	119.8	C9B—C10B—H10B	119.6
O3A—C11A—N1A	119.7 (3)	O3B—C11B—N1B	119.1 (2)

O3A—C11A—C12A	122.8 (2)	O3B—C11B—C12B	122.5 (2)
N1A—C11A—C12A	117.4 (2)	N1B—C11B—C12B	118.3 (2)
O4A—C12A—C11A	109.9 (2)	O4B—C12B—C19B	105.83 (19)
O4A—C12A—C19A	106.4 (2)	O4B—C12B—C11B	108.79 (19)
C11A—C12A—C19A	108.4 (2)	C19B—C12B—C11B	109.9 (2)
O4A—C12A—H12A	110.7	O4B—C12B—H12B	110.7
C11A—C12A—H12A	110.7	C19B—C12B—H12B	110.7
C19A—C12A—H12A	110.7	C11B—C12B—H12B	110.7
O4A—C13A—C14A	124.6 (2)	O4B—C13B—C14B	124.7 (2)
O4A—C13A—C18A	115.1 (2)	O4B—C13B—C18B	114.6 (2)
C14A—C13A—C18A	120.2 (3)	C14B—C13B—C18B	120.7 (2)
C13A—C14A—C15A	119.1 (3)	C13B—C14B—C15B	119.1 (3)
C13A—C14A—H14A	120.5	C13B—C14B—H14B	120.5
C15A—C14A—H14A	120.5	C15B—C14B—H14B	120.5
C16A—C15A—C14A	120.9 (3)	C16B—C15B—C14B	120.8 (3)
C16A—C15A—H15A	119.6	C16B—C15B—H15B	119.6
C14A—C15A—H15A	119.6	C14B—C15B—H15B	119.6
C17A—C16A—C15A	119.1 (3)	C15B—C16B—C17B	119.4 (3)
C17A—C16A—H16A	120.4	C15B—C16B—H16B	120.3
C15A—C16A—H16A	120.4	C17B—C16B—H16B	120.3
C18A—C17A—C16A	121.1 (3)	C18B—C17B—C16B	120.8 (2)
C18A—C17A—H17A	119.5	C18B—C17B—H17B	119.6
C16A—C17A—H17A	119.5	C16B—C17B—H17B	119.6
C17A—C18A—C13A	119.6 (3)	C17B—C18B—C13B	119.2 (3)
C17A—C18A—H18A	120.2	C17B—C18B—H18B	120.4
C13A—C18A—H18A	120.2	C13B—C18B—H18B	120.4
C12A—C19A—H19A	109.5	C12B—C19B—H19D	109.5
C12A—C19A—H19B	109.5	C12B—C19B—H19E	109.5
H19A—C19A—H19B	109.5	H19D—C19B—H19E	109.5
C12A—C19A—H19C	109.5	C12B—C19B—H19F	109.5
H19A—C19A—H19C	109.5	H19D—C19B—H19F	109.5
H19B—C19A—H19C	109.5	H19E—C19B—H19F	109.5
C11A—N1A—C3A	128.2 (2)	C3B—N1B—C11B	127.83 (19)
C11A—N1A—C1A	121.9 (2)	C3B—N1B—C1B	110.69 (18)
C3A—N1A—C1A	109.7 (2)	C11B—N1B—C1B	121.20 (19)
C3A—O1A—C2A	108.74 (19)	C3B—O1B—C2B	109.88 (18)
C13A—O4A—C12A	117.3 (2)	C13B—O4B—C12B	118.93 (19)

N1A—C1A—C2A—O1A	31.9 (2)	N1B—C1B—C2B—O1B	26.6 (2)
C4A—C1A—C2A—O1A	−85.1 (3)	C4B—C1B—C2B—O1B	−92.1 (2)
N1A—C1A—C2A—C5A	153.1 (2)	N1B—C1B—C2B—C5B	147.9 (2)
C4A—C1A—C2A—C5A	36.0 (3)	C4B—C1B—C2B—C5B	29.2 (3)
O1A—C2A—C5A—C6A	21.5 (3)	O1B—C2B—C5B—C10B	−148.3 (2)
C1A—C2A—C5A—C6A	−95.9 (3)	C1B—C2B—C5B—C10B	94.1 (3)
O1A—C2A—C5A—C10A	−159.5 (2)	O1B—C2B—C5B—C6B	31.5 (3)
C1A—C2A—C5A—C10A	83.2 (3)	C1B—C2B—C5B—C6B	−86.2 (3)
C10A—C5A—C6A—C7A	2.2 (4)	C10B—C5B—C6B—C7B	0.4 (4)
C2A—C5A—C6A—C7A	−178.7 (2)	C2B—C5B—C6B—C7B	−179.4 (2)

C5A—C6A—C7A—C8A	−1.2 (4)	C5B—C6B—C7B—C8B	−0.9 (4)
C6A—C7A—C8A—C9A	−1.1 (5)	C6B—C7B—C8B—C9B	0.5 (4)
C7A—C8A—C9A—C10A	2.2 (4)	C7B—C8B—C9B—C10B	0.4 (4)
C8A—C9A—C10A—C5A	−1.1 (4)	C6B—C5B—C10B—C9B	0.5 (4)
C6A—C5A—C10A—C9A	−1.1 (4)	C2B—C5B—C10B—C9B	−179.7 (2)
C2A—C5A—C10A—C9A	179.8 (2)	C8B—C9B—C10B—C5B	−0.9 (4)
O3A—C11A—C12A—O4A	−25.6 (3)	O3B—C11B—C12B—O4B	−14.6 (3)
N1A—C11A—C12A—O4A	157.0 (2)	N1B—C11B—C12B—O4B	169.3 (2)
O3A—C11A—C12A—C19A	90.2 (3)	O3B—C11B—C12B—C19B	100.8 (3)
N1A—C11A—C12A—C19A	−87.1 (3)	N1B—C11B—C12B—C19B	−75.3 (3)
O4A—C13A—C14A—C15A	−179.2 (2)	O4B—C13B—C14B—C15B	179.8 (2)
C18A—C13A—C14A—C15A	0.4 (4)	C18B—C13B—C14B—C15B	−0.2 (4)
C13A—C14A—C15A—C16A	−0.4 (4)	C13B—C14B—C15B—C16B	0.0 (4)
C14A—C15A—C16A—C17A	0.4 (4)	C14B—C15B—C16B—C17B	0.2 (4)
C15A—C16A—C17A—C18A	−0.3 (5)	C15B—C16B—C17B—C18B	−0.2 (4)
C16A—C17A—C18A—C13A	0.2 (5)	C16B—C17B—C18B—C13B	0.0 (4)
O4A—C13A—C18A—C17A	179.3 (3)	O4B—C13B—C18B—C17B	−179.8 (2)
C14A—C13A—C18A—C17A	−0.3 (4)	C14B—C13B—C18B—C17B	0.2 (4)
O3A—C11A—N1A—C3A	176.5 (2)	O2B—C3B—N1B—C11B	0.3 (4)
C12A—C11A—N1A—C3A	−6.0 (4)	O1B—C3B—N1B—C11B	179.7 (2)
O3A—C11A—N1A—C1A	−9.3 (3)	O2B—C3B—N1B—C1B	−173.6 (3)
C12A—C11A—N1A—C1A	168.2 (2)	O1B—C3B—N1B—C1B	5.8 (3)
O2A—C3A—N1A—C11A	4.0 (4)	O3B—C11B—N1B—C3B	175.9 (2)
O1A—C3A—N1A—C11A	−176.5 (2)	C12B—C11B—N1B—C3B	−7.8 (4)
O2A—C3A—N1A—C1A	−170.8 (3)	O3B—C11B—N1B—C1B	−10.8 (3)
O1A—C3A—N1A—C1A	8.7 (3)	C12B—C11B—N1B—C1B	165.5 (2)
C4A—C1A—N1A—C11A	−80.3 (3)	C4B—C1B—N1B—C3B	101.5 (2)
C2A—C1A—N1A—C11A	159.3 (2)	C2B—C1B—N1B—C3B	−20.7 (2)
C4A—C1A—N1A—C3A	94.9 (2)	C4B—C1B—N1B—C11B	−72.9 (3)
C2A—C1A—N1A—C3A	−25.5 (2)	C2B—C1B—N1B—C11B	165.0 (2)
O2A—C3A—O1A—C2A	−166.6 (2)	O2B—C3B—O1B—C2B	−167.2 (2)
N1A—C3A—O1A—C2A	13.9 (3)	N1B—C3B—O1B—C2B	13.4 (3)
C5A—C2A—O1A—C3A	−155.78 (19)	C5B—C2B—O1B—C3B	−152.58 (19)
C1A—C2A—O1A—C3A	−29.7 (2)	C1B—C2B—O1B—C3B	−26.0 (2)
C14A—C13A—O4A—C12A	11.1 (4)	C14B—C13B—O4B—C12B	−4.8 (3)
C18A—C13A—O4A—C12A	−168.4 (2)	C18B—C13B—O4B—C12B	175.3 (2)
C11A—C12A—O4A—C13A	−80.0 (3)	C19B—C12B—O4B—C13B	169.2 (2)
C19A—C12A—O4A—C13A	162.8 (2)	C11B—C12B—O4B—C13B	−72.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1*A*—H1*A*···O3*B*	1.00	2.61	3.373 (3)	133
C1*B*—H1*B*···O3*A*	1.00	2.57	3.568 (3)	174
C18*A*—H18*A*···O4*B*^{i}	0.95	2.52	3.445 (4)	165
C18*B*—H18*B*···O4*A*^{ii}	0.95	2.69	3.564 (4)	154

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