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N-Cinnamoyl-L-phenylalanine methyl ester

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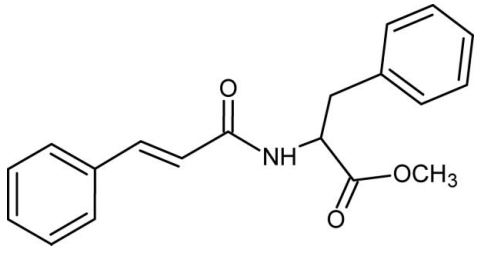
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; R factor = 0.041; wR factor = 0.125; data-to-parameter ratio = 8.4.

As part of an ongoing investigation into the development of *N*-substituted amino acids as building blocks for dynamic combinatorial chemistry, we report the structure of the title compound, $C_{19}H_{19}NO_3$. This compound crystallizes as discrete molecules. The cinnamoyl group is non-planar, with the phenyl ring and the amide twisted out of the ethylene plane. The benzyl and ester groups lie above and below the amide plane. The molecules stack along the crystallographic c axis, connecting through $C(4)$ chains of N—H···O hydrogen bonds, with the extended structure stabilized by C—H···O interactions and π–π interactions [centroid-to-centroid distances 3.547 (8) and 3.536 (8) Å].

Related literature

For related literature, see: Bernstein *et al.* (1995); Bornaghi *et al.* (2004, 2005, 2007); Poulsen *et al.* (2003).



Experimental

Crystal data

$C_{19}H_{19}NO_3$
M_r = 309.35
Orthorhombic, $P2_12_12_1$
a = 15.041 (3) Å
b = 22.550 (4) Å
c = 4.9896 (15) Å
V = 1692.4 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295.1 K
0.50 × 0.30 × 0.30 mm

Data collection

Rigaku AFC-7*R* diffractometer
Absorption correction: none
2291 measured reflections
1757 independent reflections
972 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.018
3 standard reflections
every 150 reflections
intensity decay: 0.6%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.125
S = 0.94
1757 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Selected torsion angles (°).

C9—N1—C10—C18	−82.0 (5)	C7—C8—C9—N1	−165.1 (4)
C2—C1—C7—C8	22.1 (7)	C10—C11—C12—C13	89.9 (5)
C7—C8—C9—O1	16.7 (7)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.84	2.21	3.042 (4)	169
C7—H7···O1	0.93	2.57	2.876 (5)	100

Symmetry code: (i) $x, y, z+1$.

Data collection: *MSC/AFC7 Diffractometer Control Software* (Molecular Structure Corporation, 1999); cell refinement: *MSC/AFC7 Diffractometer Control Software*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *CrystalStructure*; program(s) used to refine structure: *CrystalStructure* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2217).

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supporting information

Acta Cryst. (2008). E**64**, o139 [https://doi.org/10.1107/S1600536807055973]

N-Cinnamoyl-L-phenylalanine methyl ester

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S1. Comment

In a previous paper we reported the structure of N-cinnamoyl-*L*-valine methyl ester (Bornaghi *et al.*, 2007). This work is part of an ongoing investigation in the development of N-substituted amino acids as building blocks for dynamic combinatorial chemistry (Poulsen *et al.*, 2003; Bornaghi *et al.*, 2004; Bornaghi *et al.*, 2005). In the present communication, we report the structure of *N*-cinnamoyl-*L*-phenylalanine methyl ester.

The molecular structure of the title compound is shown in Fig. 1. Unlike the *L*-valine analogue (Bornaghi *et al.*, 2007), the cinnamoyl portion of the molecule is not planar, with the torsion angles C2—C1—C7—C8 = 22.1 (7) and C7—C8—C9—O1 = 16.7 (7)°. The benzyl and ester groups lie above and below the amide plane. The molecules stack along the short crystallographic *c* axis, connecting through C(4) chains of N—H···O hydrogen bonds (Bernstein *et al.*, 1995) (Fig. 2, Table 2). The macro structure is stabilized by short C—H···O contact interactions between the molecules in stacks and with adjacent neighbours. Fig. 3 displays how the molecular stacks interlock about the benzyl group. The stacks are held in close proximity through the short contact O1···H15^{ii} = 2.7 Å [symmetry code ii: -*x* + 1/2, -*y* + 1, *z* - 1/2]. Adjacent macro structures are oriented about the ester group through π interactions with benzyl rings (C13···C17^{v} = 3.547 (8) and C14···C16^{v} = 3.536 (8) Å) [symmetry code v: *x*, *y*, *z* + 1] and C—H···O interactions with the cinnamoyl rings.

S2. Experimental

Triethylamine (0.93 g, 9.2 mmol) was added dropwise to a solution of *L*-phenylalanine methyl ester hydrochloride (0.5 g, 2.3 mmol) and cinnamoyl chloride (367 mg, 2.2 mmol) in anhydrous dichloromethane (10 ml). The reaction mixture was stirred at room temperature (298 K) for 3 days before being washed with 2 *M* HCl (2 *x* 100 ml), and saturated brine solution (100 ml), then dried over $MgSO_4$. Solvent was removed under reduced pressure to give a clear solid residue. The title compound was obtained in 83% yield after crystallization from an ethyl acetate/hexane solution. ^{1}H NMR ($CDCl_3$, 300 MHz, p.p.m.): δ = 3.07–3.21 (m, 2H, βCH), 3.67 (s, 3H, OCH_3), 4.95–5.01 (m, 1H, αCH), 6.10 (br d, 1H, NH), 6.33 (d, 1H, J = 15.6 Hz, ?CHCO), 7.03–7.50 (m, 10H, ArH), 7.57 (d, 1H, J =15.6 Hz, ?CHPh); ^{13}C NMR ($CDCl_3$, 75 MHz, p.p.m.): δ = 37.9 (βCH), 52.5 (OCH_3), 53.3 (αCH), 119.9 (?CHCO), 127.2, 127.9, 128.4, 128.9, 129.4, 129.9, 130.7 (CH from Ar), 134.6, 135.8 (C from Ar), 142.0 (?CHPh), 165.4 (CONH), 172.1 ($COOCH_3$); MS (LRMSES): m/*z* 310.0 [*M*+H]$^+$, 332.1 [*M*+Na]$^+$; mp 361.8 K.

S3. Refinement

H1 attached to N1 and H10 attached to C10 were located in Fourier maps and constrained with N—H = 0.84 and C—H = 0.98 Å respectively. All other H atoms were placed in calculated positions and constrained as riding with C—H = 0.93–0.97 Å. In the absence of significant anomalous scattering effects, Friedel pairs were merged. The absolute configuration of the title compound was assigned on the basis of the known configuration of the starting material.

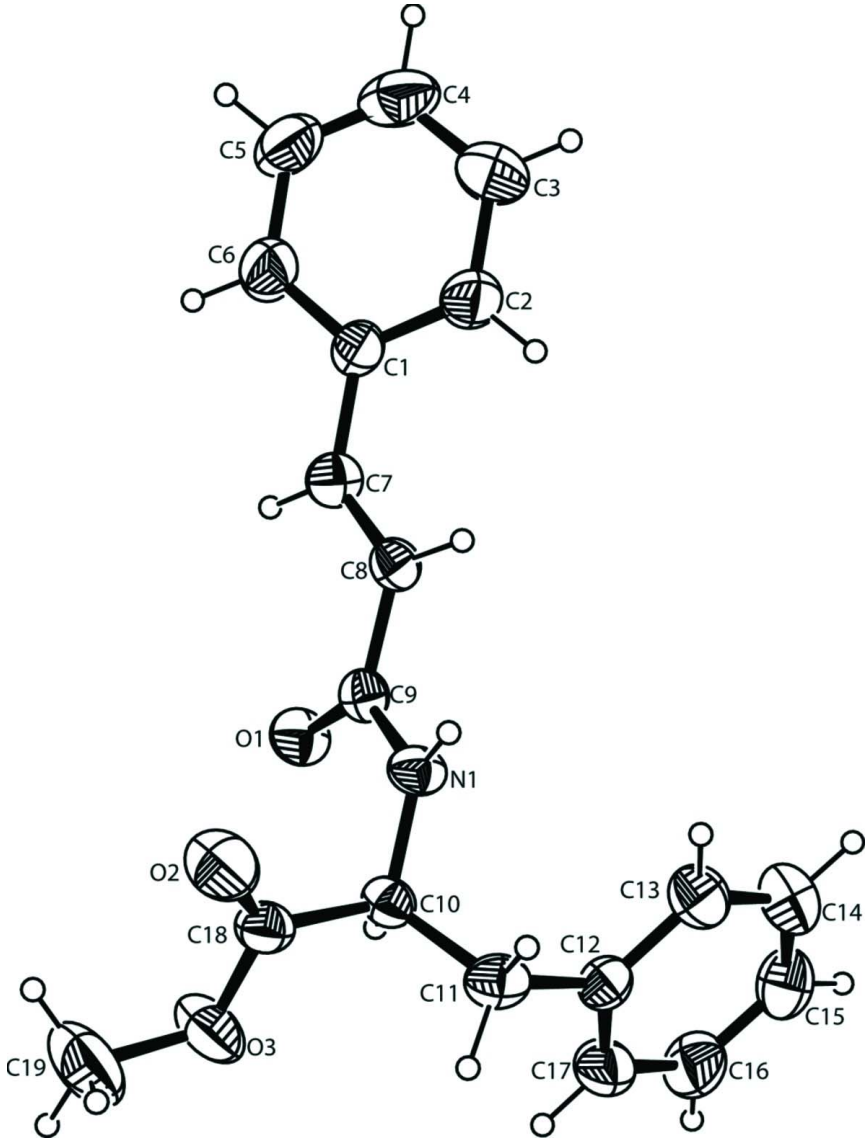

Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. H atoms are included as spheres of arbitrary radius.

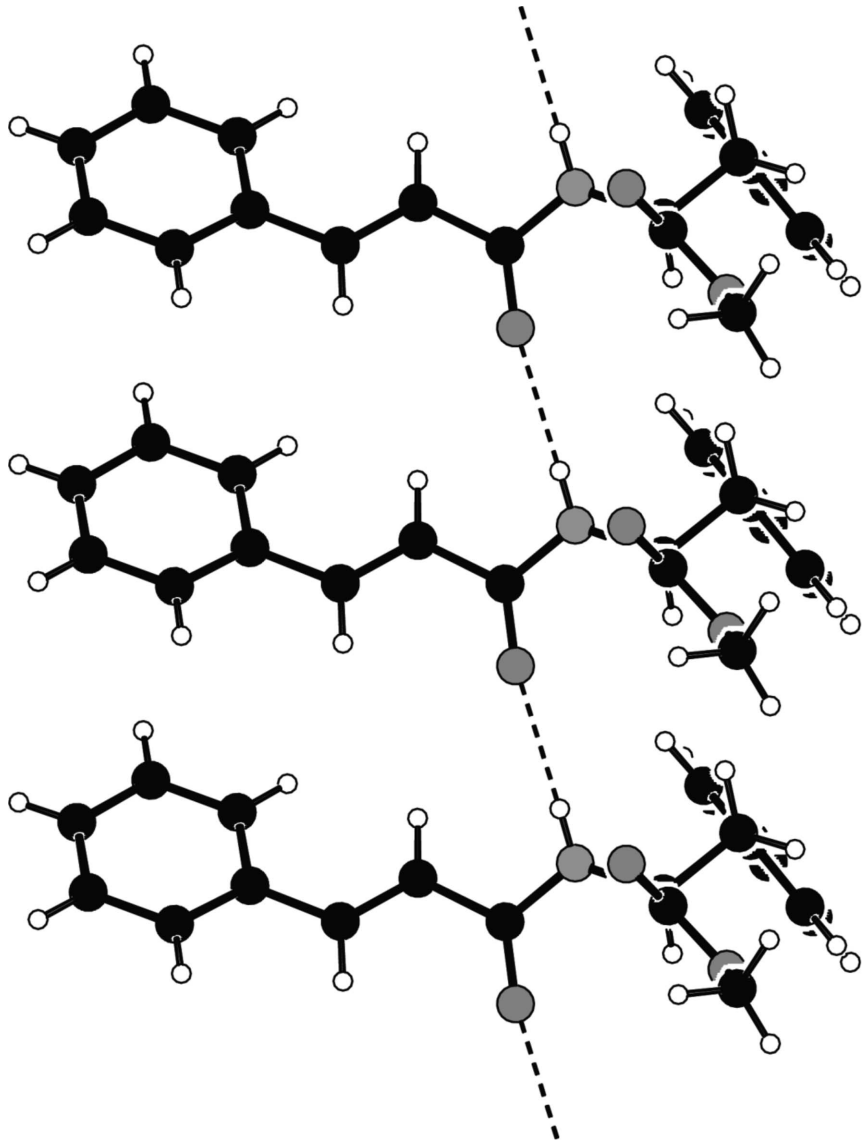

Figure 2

View of the C(4) N—H···O hydrogen bonding along the *c* axis. Hydrogen bonding is shown with dashed lines.

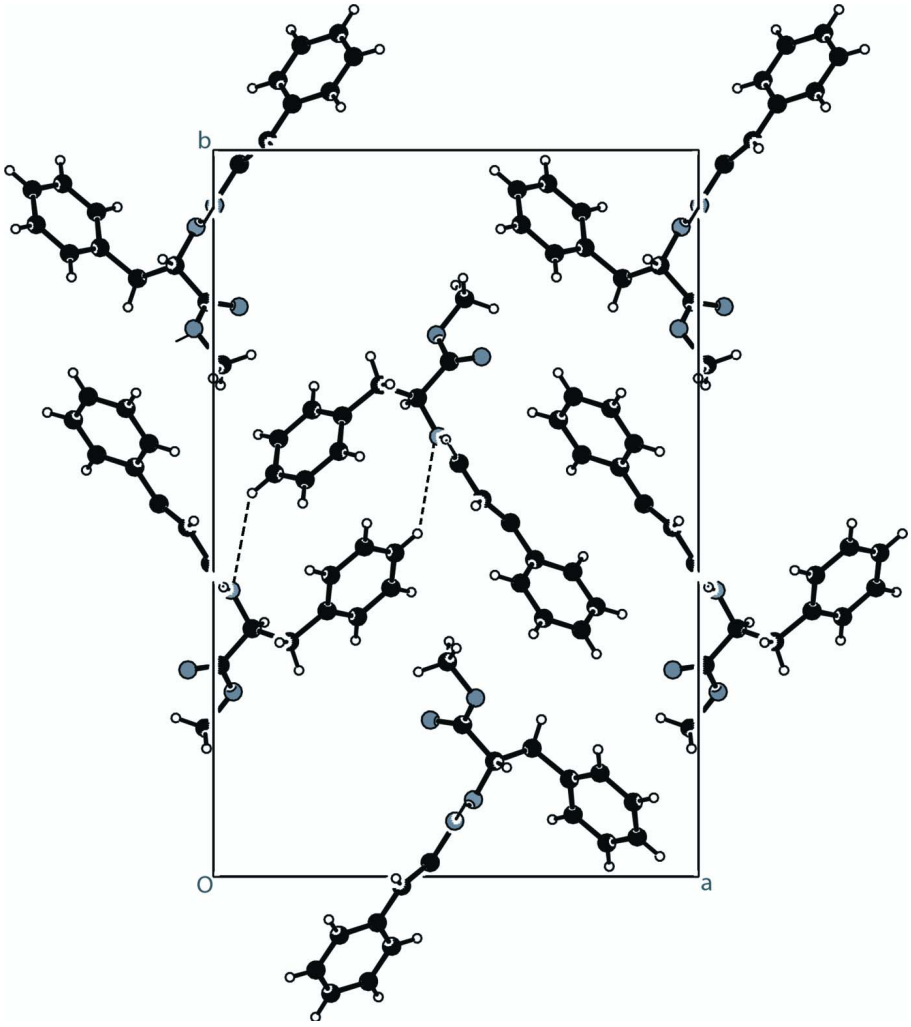

Figure 3

View of the crystal packing projected on to the *ab* plane. Hydrogen bonding is shown with dashed lines.

N-Cinnamoyl-*L*-phenylalanine methyl ester

Crystal data

$C_{19}H_{19}NO_3$
$M_r = 309.35$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 15.041\ (3)$ Å
$b = 22.550\ (4)$ Å
$c = 4.9896\ (15)$ Å
$V = 1692.4\ (7)$ Å^3
$Z = 4$
$F(000) = 656.00$
$D_x = 1.214$ Mg m^{-3}
Melting point: 361.8 K
Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å
Cell parameters from 20 reflections
$\theta = 9.8$–$10.0°$
$\mu = 0.08$ mm^{-1}
$T = 295$ K
Prismatic, colourless
0.50 × 0.30 × 0.30 mm

Data collection

Rigaku AFC7R diffractometer
Radiation source: Rigaku rotating anode
Graphite monochromator
ω scans
2291 measured reflections
1757 independent reflections
972 reflections with $F^2 > 2\sigma(F^2)$
$R_{int} = 0.018$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$
$h = -8 \rightarrow 17$
$k = 0 \rightarrow 26$
$l = -5 \rightarrow 2$
3 standard reflections every 150 reflections
intensity decay: 0.6%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.125$
$S = 0.94$
1757 reflections
209 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Special details

Experimental. The scan width was (0.89 + 0.30tanθ)° with an ω scan speed of 16° per minute (up to 4 scans to achieve I/σ(I) > 10). Stationary background counts were recorded at each end of the scan, and the scan time:background time ratio was 2:1.

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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}
O1	0.5025 (2)	0.57628 (13)	0.1198 (6)	0.0679 (11)
O2	0.5528 (2)	0.71550 (16)	0.5337 (8)	0.0997 (14)
O3	0.4596 (2)	0.74577 (14)	0.2226 (8)	0.1010 (14)
N1	0.4640 (2)	0.60588 (14)	0.5364 (6)	0.0571 (11)
C1	0.6624 (3)	0.43634 (19)	0.4699 (10)	0.0617 (17)
C2	0.6329 (3)	0.4040 (2)	0.6869 (12)	0.0847 (19)
C3	0.6806 (4)	0.3555 (2)	0.7816 (15)	0.108 (3)
C4	0.7582 (4)	0.3394 (2)	0.6570 (17)	0.107 (3)
C5	0.7888 (4)	0.3713 (3)	0.4499 (16)	0.103 (3)
C6	0.7406 (3)	0.4194 (2)	0.3554 (12)	0.088 (2)
C7	0.6124 (3)	0.48703 (18)	0.3641 (9)	0.0623 (17)
C8	0.5533 (3)	0.51934 (17)	0.4910 (9)	0.0543 (14)
C9	0.5062 (3)	0.56890 (18)	0.3631 (9)	0.0520 (14)
C10	0.4203 (3)	0.65879 (17)	0.4456 (9)	0.0543 (16)

C11	0.3434 (3)	0.67665 (17)	0.6256 (10)	0.0657 (17)
C12	0.2658 (3)	0.63417 (19)	0.6032 (10)	0.0583 (17)
C13	0.2587 (3)	0.5853 (2)	0.7655 (10)	0.0763 (17)
C14	0.1888 (4)	0.5462 (2)	0.7362 (12)	0.093 (2)
C15	0.1263 (3)	0.5546 (2)	0.5393 (12)	0.084 (2)
C16	0.1342 (3)	0.6024 (3)	0.3770 (12)	0.094 (2)
C17	0.2032 (3)	0.6424 (2)	0.4064 (12)	0.0817 (19)
C18	0.4866 (3)	0.70907 (19)	0.4097 (10)	0.0627 (17)
C19	0.5177 (4)	0.7956 (2)	0.1654 (14)	0.138 (3)
H1	0.47910	0.60170	0.69710	0.0640*
H2	0.58020	0.41490	0.77140	0.1020*
H3	0.65990	0.33410	0.92820	0.1300*
H4	0.78960	0.30640	0.71620	0.1290*
H5	0.84250	0.36120	0.36950	0.1240*
H6	0.76220	0.44070	0.20960	0.1050*
H7	0.62380	0.49740	0.18710	0.0750*
H8	0.54080	0.51050	0.66920	0.0650*
H10	0.39530	0.65010	0.26850	0.0650*
H13	0.30150	0.57840	0.89650	0.0920*
H14	0.18390	0.51390	0.85110	0.1110*
H15	0.07960	0.52790	0.51790	0.1010*
H16	0.09220	0.60850	0.24280	0.1130*
H17	0.20720	0.67490	0.29260	0.0980*
H111	0.36370	0.67780	0.81010	0.0780*
H112	0.32380	0.71620	0.57730	0.0780*
H191	0.57770	0.78170	0.14720	0.1660*
H192	0.51440	0.82370	0.30950	0.1660*
H193	0.49930	0.81420	0.00160	0.1660*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.088 (2)	0.079 (2)	0.0367 (17)	0.0117 (18)	0.0021 (17)	0.0012 (17)
O2	0.085 (2)	0.095 (2)	0.119 (3)	−0.021 (2)	−0.039 (3)	0.023 (3)
O3	0.107 (2)	0.082 (2)	0.114 (3)	−0.021 (2)	−0.033 (3)	0.045 (2)
N1	0.071 (2)	0.060 (2)	0.0402 (18)	0.015 (2)	−0.0017 (18)	0.0019 (18)
C1	0.055 (3)	0.056 (3)	0.074 (3)	−0.002 (2)	0.007 (3)	−0.006 (3)
C2	0.078 (3)	0.063 (3)	0.113 (4)	0.010 (3)	0.016 (3)	0.003 (3)
C3	0.118 (5)	0.071 (4)	0.136 (6)	0.017 (4)	0.007 (5)	0.021 (4)
C4	0.084 (4)	0.069 (4)	0.169 (7)	0.018 (3)	−0.021 (5)	−0.008 (5)
C5	0.066 (3)	0.086 (4)	0.158 (7)	0.012 (3)	0.012 (4)	−0.004 (5)
C6	0.082 (4)	0.074 (3)	0.107 (4)	0.005 (3)	0.025 (4)	0.002 (4)
C7	0.066 (3)	0.065 (3)	0.056 (3)	0.004 (3)	0.000 (3)	−0.004 (3)
C8	0.060 (3)	0.056 (2)	0.047 (2)	−0.001 (2)	0.001 (2)	0.003 (2)
C9	0.056 (3)	0.049 (2)	0.051 (2)	−0.005 (2)	0.001 (2)	−0.003 (2)
C10	0.058 (3)	0.052 (2)	0.053 (3)	0.000 (2)	−0.006 (2)	0.005 (2)
C11	0.078 (3)	0.058 (3)	0.061 (3)	0.012 (2)	−0.003 (3)	−0.013 (3)
C12	0.059 (3)	0.061 (3)	0.055 (3)	0.005 (2)	0.007 (3)	−0.007 (3)

C13	0.088 (3)	0.075 (3)	0.066 (3)	−0.004 (3)	−0.002 (3)	0.003 (3)
C14	0.106 (4)	0.083 (3)	0.089 (4)	−0.017 (3)	0.004 (4)	0.014 (4)
C15	0.072 (3)	0.093 (4)	0.088 (4)	−0.022 (3)	0.006 (4)	−0.010 (4)
C16	0.060 (3)	0.119 (4)	0.102 (4)	−0.006 (3)	−0.012 (3)	0.014 (4)
C17	0.069 (3)	0.085 (3)	0.091 (4)	0.002 (3)	−0.011 (3)	0.024 (4)
C18	0.063 (3)	0.060 (3)	0.065 (3)	0.007 (3)	−0.006 (3)	0.007 (3)
C19	0.151 (6)	0.089 (4)	0.175 (7)	−0.044 (4)	−0.027 (6)	0.052 (5)

Geometric parameters (Å, º)

O1—C9	1.227 (5)	C14—C15	1.373 (8)
O2—C18	1.181 (6)	C15—C16	1.353 (8)
O3—C18	1.312 (6)	C16—C17	1.383 (7)
O3—C19	1.452 (6)	C2—H2	0.9300
N1—C9	1.359 (5)	C3—H3	0.9300
N1—C10	1.436 (5)	C4—H4	0.9300
N1—H1	0.8400	C5—H5	0.9300
C1—C6	1.362 (7)	C6—H6	0.9300
C1—C7	1.467 (6)	C7—H7	0.9300
C1—C2	1.379 (7)	C8—H8	0.9300
C2—C3	1.391 (7)	C10—H10	0.9800
C3—C4	1.371 (9)	C11—H111	0.9700
C4—C5	1.341 (10)	C11—H112	0.9700
C5—C6	1.387 (8)	C13—H13	0.9300
C7—C8	1.312 (6)	C14—H14	0.9300
C8—C9	1.469 (6)	C15—H15	0.9300
C10—C11	1.519 (6)	C16—H16	0.9300
C10—C18	1.521 (6)	C17—H17	0.9300
C11—C12	1.514 (6)	C19—H191	0.9600
C12—C17	1.373 (7)	C19—H192	0.9600
C12—C13	1.372 (7)	C19—H193	0.9600
C13—C14	1.380 (7)		
O1···N1^{i}	3.042 (4)	H1···O2	2.9100
O1···C18	3.334 (5)	H1···H8	2.2600
O2···N1	2.810 (5)	H1···H111	2.5100
O1···H1^{i}	2.2100	H2···C8	2.7700
O1···H7	2.5700	H2···H8	2.2900
O1···H10	2.4300	H4···O2^{iv}	2.8900
O1···H15^{ii}	2.7000	H5···O2^{iii}	2.8800
O1···H8^{i}	2.7500	H6···H7	2.4500
O2···H1	2.9100	H6···C7^{iii}	3.0300
O2···H191	2.4700	H7···O1	2.5700
O2···H192	2.7500	H7···H6	2.4500
O2···H4^{iii}	2.8900	H8···O1^{v}	2.7500
O2···H5^{iv}	2.8800	H8···C2	2.7700
O3···H112	2.7800	H8···H1	2.2600
N1···O1^{v}	3.042 (4)	H8···H2	2.2900

N1···O2	2.810 (5)	H10···O1	2.4300
N1···C13	3.325 (6)	H10···C17	2.9800
C3···C6^{v}	3.330 (9)	H10···H111^{i}	2.4200
C6···C3^{i}	3.330 (9)	H13···H111	2.4700
C13···C17^{v}	3.547 (8)	H14···C14^{viii}	3.0300
C13···N1	3.325 (6)	H15···O1^{viii}	2.7000
C14···C16^{v}	3.536 (8)	H15···C9^{viii}	3.0700
C16···C14^{i}	3.536 (8)	H16···H193^{ix}	2.5500
C17···C13^{i}	3.547 (8)	H17···H112	2.4400
C18···O1	3.334 (5)	H111···H1	2.5100
C2···H193^{vi}	2.9900	H111···H10^{v}	2.4200
C2···H8	2.7700	H111···H13	2.4700
C7···H6^{iv}	3.0300	H112···O3	2.7800
C8···H2	2.7700	H112···H17	2.4400
C9···H15^{ii}	3.0700	H191···O2	2.4700
C14···H14^{ii}	3.0300	H192···O2	2.7500
C16···H192^{vii}	2.9100	H192···C16^{x}	2.9100
C17···H10	2.9800	H193···H16^{xi}	2.5500
H1···O1^{v}	2.2100	H193···C2^{xii}	2.9900

C18—O3—C19	116.2 (4)	C4—C3—H3	120.00
C9—N1—C10	121.5 (3)	C3—C4—H4	120.00
C10—N1—H1	121.00	C5—C4—H4	120.00
C9—N1—H1	114.00	C4—C5—H5	120.00
C2—C1—C7	122.0 (4)	C6—C5—H5	120.00
C6—C1—C7	120.7 (4)	C1—C6—H6	119.00
C2—C1—C6	117.3 (4)	C5—C6—H6	119.00
C1—C2—C3	121.1 (5)	C1—C7—H7	116.00
C2—C3—C4	119.6 (6)	C8—C7—H7	116.00
C3—C4—C5	120.0 (5)	C7—C8—H8	119.00
C4—C5—C6	120.1 (6)	C9—C8—H8	119.00
C1—C6—C5	121.9 (5)	N1—C10—H10	107.00
C1—C7—C8	127.3 (4)	C11—C10—H10	107.00
C7—C8—C9	122.7 (4)	C18—C10—H10	107.00
N1—C9—C8	114.6 (4)	C10—C11—H111	109.00
O1—C9—N1	121.7 (4)	C10—C11—H112	109.00
O1—C9—C8	123.7 (4)	C12—C11—H111	109.00
C11—C10—C18	111.8 (3)	C12—C11—H112	109.00
N1—C10—C18	110.9 (4)	H111—C11—H112	108.00
N1—C10—C11	112.5 (3)	C12—C13—H13	120.00
C10—C11—C12	112.1 (4)	C14—C13—H13	120.00
C11—C12—C13	121.7 (4)	C13—C14—H14	120.00
C11—C12—C17	119.7 (4)	C15—C14—H14	120.00
C13—C12—C17	118.5 (4)	C14—C15—H15	121.00
C12—C13—C14	120.7 (5)	C16—C15—H15	121.00
C13—C14—C15	120.6 (5)	C15—C16—H16	119.00
C14—C15—C16	118.6 (4)	C17—C16—H16	119.00
C15—C16—C17	121.5 (5)	C12—C17—H17	120.00

C12—C17—C16	120.2 (5)	C16—C17—H17	120.00
O3—C18—C10	110.6 (4)	O3—C19—H191	109.00
O2—C18—O3	123.8 (4)	O3—C19—H192	109.00
O2—C18—C10	125.6 (4)	O3—C19—H193	109.00
C1—C2—H2	119.00	H191—C19—H192	110.00
C3—C2—H2	120.00	H191—C19—H193	109.00
C2—C3—H3	120.00	H192—C19—H193	110.00

C19—O3—C18—O2	1.9 (7)	C7—C8—C9—N1	−165.1 (4)
C19—O3—C18—C10	−179.2 (4)	N1—C10—C11—C12	−70.0 (5)
C10—N1—C9—O1	−6.3 (6)	C18—C10—C11—C12	164.5 (4)
C10—N1—C9—C8	175.5 (4)	N1—C10—C18—O2	−30.1 (6)
C9—N1—C10—C11	151.9 (4)	N1—C10—C18—O3	151.0 (4)
C9—N1—C10—C18	−82.0 (5)	C11—C10—C18—O2	96.3 (6)
C6—C1—C2—C3	−1.0 (8)	C11—C10—C18—O3	−82.6 (5)
C7—C1—C2—C3	179.0 (5)	C10—C11—C12—C13	89.9 (5)
C2—C1—C6—C5	0.6 (8)	C10—C11—C12—C17	−86.4 (5)
C7—C1—C6—C5	−179.4 (5)	C11—C12—C13—C14	−178.0 (5)
C2—C1—C7—C8	22.1 (7)	C17—C12—C13—C14	−1.8 (7)
C6—C1—C7—C8	−157.9 (5)	C11—C12—C17—C16	177.2 (5)
C1—C2—C3—C4	−0.2 (9)	C13—C12—C17—C16	0.9 (7)
C2—C3—C4—C5	1.8 (10)	C12—C13—C14—C15	1.8 (8)
C3—C4—C5—C6	−2.2 (10)	C13—C14—C15—C16	−0.8 (8)
C4—C5—C6—C1	1.0 (10)	C14—C15—C16—C17	−0.1 (8)
C1—C7—C8—C9	−179.2 (4)	C15—C16—C17—C12	0.1 (8)
C7—C8—C9—O1	16.7 (7)		

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) −*x*+1/2, −*y*+1, *z*−1/2; (iii) −*x*+3/2, −*y*+1, *z*−1/2; (iv) −*x*+3/2, −*y*+1, *z*+1/2; (v) *x*, *y*, *z*+1; (vi) −*x*+1, *y*−1/2, −*z*+1/2; (vii) *x*−1/2, −*y*+3/2, −*z*+1; (viii) −*x*+1/2, −*y*+1, *z*+1/2; (ix) *x*−1/2, −*y*+3/2, −*z*; (x) *x*+1/2, −*y*+3/2, −*z*+1; (xi) *x*+1/2, −*y*+3/2, −*z*; (xii) −*x*+1, *y*+1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{v}	0.84	2.21	3.042 (4)	169
C7—H7···O1	0.93	2.57	2.876 (5)	100

Symmetry code: (v) *x*, *y*, *z*+1.