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1-(4-Methylphenyl)-5-oxo-2-phenylpyrrolidine-2-carboxamide–methanol (1/1)

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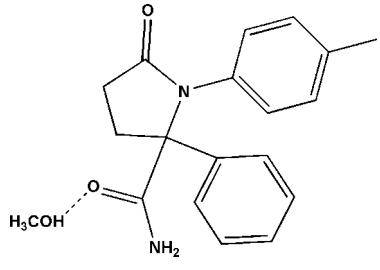
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.110; data-to-parameter ratio = 14.6.

1-(4-Methylphenyl)-5-oxo-2-phenylpyrrolidine-2-carboxamide is a potential anti-human immunodeficiency virus type 1 (HIV-1) non-nucleoside reverse transcriptase inhibitor. In the title compound, $C_{18}H_{18}N_2O_2{\cdot}CH_4O$, the pyrrolidine ring has a well expressed envelope conformation. The 1-(4-methylphenyl)-5-oxo-2-phenylpyrrolidine-2-carboxamide molecules are connected into infinite chains *via* hydrogen bonding with CH_3OH solvent molecules.

Related literature

For details of the synthesis, see: Martirosyan *et al.* (2000, 2004). For details of the pharmacological properties of compounds of this family, see: De Clercq (1996). For the crystal structures of some analogs of the title compound, see: Karapetyan *et al.* (2002) and Tamazyan *et al.* (2002).



Experimental

Crystal data

$C_{18}H_{18}N_2O_2{\cdot}CH_4O$
M_r = 326.39
Monoclinic, $P2_1/n$
a = 7.9421 (16) Å
b = 20.761 (4) Å
c = 10.403 (2) Å
β = 94.47 (3)°
V = 1710.2 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.35 × 0.28 × 0.23 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
8228 measured reflections
4122 independent reflections
2990 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
3 standard reflections
frequency: 180 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.110
S = 1.02
4122 reflections
283 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3o···O2	0.84 (2)	1.90 (2)	2.741 (2)	176 (2)
N2^{i}—H2nB^{i}···O3	0.91 (2)	2.00 (2)	2.860 (2)	156 (2)

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *CAD-4 DATCOL* (Enraf–Nonius, 1988); cell refinement: *CAD-4 LS* (Enraf–Nonius, 1988); data reduction: *HELENA* (Spek, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-NT* (Bruker, 2000) and *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXTL-NT*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2158).

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supplementary materials

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1-(4-Methylphenyl)-5-oxo-2-phenylpyrrolidine-2-carboxamide-methanol (1/1)

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Comment

The interest in the X-ray structural investigation of the title compound is stimulated by their potential HIV-1 RT inhibition properties (De Clercq, 1996). These compounds belong to a family of non-nucleoside reverse transcriptase inhibitors (NNRTIs). Related structures have been published by Karapetyan *et al.*, 2002 and Tamazyan, *et al.*, 2002.

A view of the molecule with our numbering scheme is depicted in Fig. 1. A ll intramolecular interatomic distances are in good agreement with their mean statistical values. The crystal structure consists of infinite chains along the [10$\bar{1}$] direction of crystal lattice. These chains molecules are formed by molecules of the title compound, $C_{18}H_{18}N_2O_2$, and solvent CH_3OH molecules *via* O2···H3o—O3···H2b^{i}—N2^{i} hydrogen bonding (Fig.2).

Experimental

The title compound was synthesized by the cycloalkylation of N1-cyano(phenyl)methyl-N1-(4-methylphenyl)-3-chloropropanamide under phase-transfer catalysis conditions and then by hydrolysis in concentrated sulfuric acid as it is described by Martirosyan *et al.*, 2000, 2004. The compound as synthesized is a racemic mixture of molecules (2*R* and 2S)-1-(4-methylphenyl)-5-oxo-2-phenyltetrahydro-1H −2-pyrrolecarboxamide. The crystals were grown from a methanol solution of the compound.

Refinement

The positional parameters of H atoms besides those belonging to methyl groups were determined from difference Fourier maps. H atoms of methyl groups were positioned geometrically and refined using a riding model with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C). The positional parameters of all atoms, anisotropic thermal parameters of nonhydrogen atoms and isotropic thermal parameters of remaining hydrogen atoms were refined without restraints.

Figures

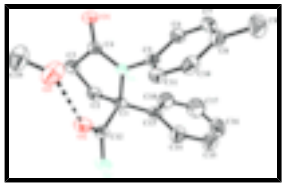

Fig. 1. A view of the molecule with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.

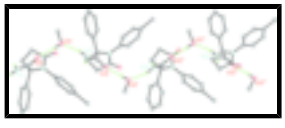

Fig. 2. The formation of infinite chain of molecules *via* hydrogen bonding. For clarity only H atoms participating in bonding are depicted. Symmetry codes: (i) 1/2 + *x*, 1/2 − *y*, −1/2 + *z*; (ii) 1 + *x*, *y*, −1 + *z*; (iii) 1.5 + *x*, 1/2 − *y*, −1.5 + *z*.

1-(4-methylphenyl)-5-oxo-2-phenylpyrrolidine-2-carboxamide –methanol (1/1)

Crystal data

$C_{18}H_{18}N_2O_2 \cdot CH_4O$	$F_{000} = 696$
$M_r = 326.39$	$D_x = 1.268$ Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 96.0 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.9421$ (16) Å	Cell parameters from 25 reflections
$b = 20.761$ (4) Å	$\theta = 10$–15^o
$c = 10.403$ (2) Å	$\mu = 0.09$ mm^{-1}
$\beta = 94.47$ (3)º	$T = 293$ (2) K
$V = 1710.2$ (6) Å^3	Prism, colourless
$Z = 4$	0.35 × 0.28 × 0.23 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.030$
Radiation source: fine-focus sealed tube	$\theta_{max} = 28.0^o$
Monochromator: graphite	$\theta_{min} = 2.0^o$
$T = 293$(2) K	$h = -10 \rightarrow 10$
$\theta/2\theta$ scans	$k = 0 \rightarrow 27$
Absorption correction: none	$l = -13 \rightarrow 13$
8228 measured reflections	3 standard reflections
4122 independent reflections	every 180 min
2990 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.110$	$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.3702P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
4122 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
283 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.09584 (16)	0.29428 (7)	0.70924 (12)	0.0236 (3)
N1	0.25160 (13)	0.28492 (5)	0.64212 (10)	0.0241 (2)
O1	0.46719 (12)	0.21200 (5)	0.63351 (11)	0.0363 (3)
C2	0.13038 (19)	0.24956 (8)	0.82787 (13)	0.0304 (3)
H2A	0.192 (2)	0.2739 (8)	0.8979 (16)	0.036 (4)*
H2B	0.024 (2)	0.2325 (8)	0.8585 (16)	0.041 (5)*
H2NA	−0.297 (2)	0.2556 (9)	0.6374 (18)	0.046 (5)*
H2NB	−0.222 (2)	0.3044 (9)	0.7367 (18)	0.043 (5)*
N2	−0.20793 (15)	0.27778 (7)	0.66831 (13)	0.0310 (3)
O2	−0.03691 (12)	0.22527 (5)	0.54227 (10)	0.0348 (3)
C3	0.24343 (19)	0.19719 (8)	0.77964 (15)	0.0326 (3)
H3A	0.320 (2)	0.1794 (9)	0.8450 (17)	0.042 (5)*
H3B	0.175 (2)	0.1615 (9)	0.7353 (17)	0.043 (5)*
C4	0.33748 (16)	0.23050 (7)	0.67804 (13)	0.0265 (3)
C5	0.30378 (16)	0.32782 (7)	0.54477 (13)	0.0242 (3)
C6	0.43874 (17)	0.36892 (7)	0.57445 (15)	0.0305 (3)
H6	0.493 (2)	0.3684 (8)	0.6611 (16)	0.033 (4)*
C7	0.4904 (2)	0.41026 (8)	0.48041 (16)	0.0362 (3)
H7	0.582 (2)	0.4392 (9)	0.4998 (17)	0.046 (5)*
C8	0.4083 (2)	0.41248 (7)	0.35797 (15)	0.0351 (3)
C9	0.4635 (3)	0.45847 (9)	0.25726 (19)	0.0544 (5)
H9A	0.4045	0.4986	0.2633	0.082*
H9B	0.4384	0.4403	0.1731	0.082*
H9C	0.5829	0.4658	0.2712	0.082*
C10	0.2733 (2)	0.37093 (8)	0.33059 (15)	0.0343 (3)
H10	0.215 (2)	0.3694 (8)	0.2450 (18)	0.042 (5)*
C11	0.22140 (18)	0.32872 (7)	0.42227 (14)	0.0292 (3)
H11	0.132 (2)	0.2979 (8)	0.4011 (16)	0.035 (4)*
C12	−0.05730 (16)	0.26366 (7)	0.62983 (12)	0.0243 (3)
C13	0.07342 (17)	0.36569 (7)	0.73870 (14)	0.0286 (3)
C14	−0.0165 (2)	0.40578 (8)	0.65111 (16)	0.0377 (4)
H14	−0.067 (2)	0.3876 (9)	0.5741 (19)	0.050 (5)*
C15	−0.0277 (2)	0.47155 (9)	0.6730 (2)	0.0475 (4)

H15	−0.092 (3)	0.4978 (11)	0.612 (2)	0.061 (6)*
C16	0.0504 (3)	0.49807 (9)	0.7833 (2)	0.0546 (5)
H16	0.042 (3)	0.5427 (11)	0.799 (2)	0.062 (6)*
C17	0.1403 (3)	0.45928 (10)	0.8694 (2)	0.0606 (6)
H17	0.197 (3)	0.4758 (12)	0.947 (2)	0.080 (7)*
C18	0.1530 (2)	0.39355 (9)	0.84826 (18)	0.0455 (4)
H18	0.224 (3)	0.3675 (10)	0.908 (2)	0.060 (6)*
O3	0.15641 (18)	0.15833 (7)	0.38084 (12)	0.0523 (4)
H3O	0.099 (3)	0.1805 (12)	0.430 (2)	0.078 (8)*
C19	0.2047 (3)	0.10171 (9)	0.44502 (18)	0.0544 (5)
H19A	0.2758	0.1118	0.5212	0.082*
H19B	0.2654	0.0749	0.3894	0.082*
H19C	0.1060	0.0793	0.4688	0.082*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0186 (6)	0.0312 (7)	0.0213 (6)	−0.0009 (5)	0.0034 (5)	−0.0005 (5)
N1	0.0175 (5)	0.0297 (6)	0.0253 (5)	0.0008 (4)	0.0037 (4)	0.0033 (5)
O1	0.0213 (5)	0.0366 (6)	0.0515 (6)	0.0041 (4)	0.0057 (4)	0.0027 (5)
C2	0.0288 (7)	0.0387 (8)	0.0235 (7)	−0.0044 (6)	0.0001 (6)	0.0048 (6)
N2	0.0194 (5)	0.0407 (7)	0.0334 (6)	−0.0021 (5)	0.0045 (5)	−0.0081 (6)
O2	0.0247 (5)	0.0455 (6)	0.0341 (5)	0.0002 (4)	0.0018 (4)	−0.0143 (5)
C3	0.0267 (7)	0.0361 (8)	0.0343 (8)	−0.0025 (6)	−0.0015 (6)	0.0106 (7)
C4	0.0192 (6)	0.0279 (7)	0.0318 (7)	−0.0024 (5)	−0.0028 (5)	0.0008 (6)
C5	0.0200 (6)	0.0265 (7)	0.0269 (6)	0.0034 (5)	0.0062 (5)	0.0006 (5)
C6	0.0264 (7)	0.0331 (8)	0.0321 (7)	−0.0014 (6)	0.0024 (6)	0.0010 (6)
C7	0.0317 (8)	0.0320 (8)	0.0459 (9)	−0.0056 (6)	0.0093 (7)	0.0032 (7)
C8	0.0388 (8)	0.0299 (8)	0.0386 (8)	0.0081 (6)	0.0166 (6)	0.0073 (6)
C9	0.0663 (12)	0.0456 (10)	0.0547 (11)	0.0038 (9)	0.0260 (9)	0.0187 (9)
C10	0.0392 (8)	0.0365 (8)	0.0275 (7)	0.0075 (7)	0.0042 (6)	0.0039 (6)
C11	0.0267 (7)	0.0323 (7)	0.0287 (7)	0.0005 (6)	0.0022 (5)	0.0005 (6)
C12	0.0210 (6)	0.0291 (7)	0.0230 (6)	0.0006 (5)	0.0021 (5)	0.0020 (5)
C13	0.0224 (6)	0.0324 (7)	0.0322 (7)	−0.0017 (5)	0.0093 (5)	−0.0035 (6)
C14	0.0421 (9)	0.0360 (8)	0.0359 (8)	0.0037 (7)	0.0083 (7)	−0.0008 (7)
C15	0.0505 (10)	0.0371 (9)	0.0570 (11)	0.0067 (8)	0.0173 (9)	0.0043 (8)
C16	0.0558 (11)	0.0317 (9)	0.0786 (14)	−0.0040 (8)	0.0191 (10)	−0.0131 (9)
C17	0.0626 (13)	0.0473 (12)	0.0702 (14)	−0.0063 (10)	−0.0055 (11)	−0.0251 (10)
C18	0.0433 (9)	0.0416 (10)	0.0501 (10)	−0.0011 (8)	−0.0055 (8)	−0.0125 (8)
O3	0.0678 (9)	0.0518 (8)	0.0404 (7)	0.0186 (7)	0.0246 (6)	0.0102 (6)
C19	0.0786 (14)	0.0398 (10)	0.0466 (10)	0.0067 (9)	0.0168 (9)	0.0003 (8)

Geometric parameters (Å, °)

C1—N1	1.4800 (16)	C8—C9	1.508 (2)
C1—C13	1.527 (2)	C9—H9A	0.9600
C1—C2	1.5517 (19)	C9—H9B	0.9600
C1—C12	1.5522 (18)	C9—H9C	0.9600
N1—C4	1.3571 (17)	C10—C11	1.382 (2)

N1—C5	1.4338 (17)	C10—H10	0.973 (18)
O1—C4	1.2238 (17)	C11—H11	0.967 (17)
C2—C3	1.520 (2)	C13—C18	1.386 (2)
C2—H2A	0.985 (17)	C13—C14	1.390 (2)
C2—H2B	0.995 (18)	C14—C15	1.388 (2)
N2—C12	1.3236 (17)	C14—H14	0.947 (19)
N2—H2NA	0.88 (2)	C15—C16	1.376 (3)
N2—H2NB	0.915 (19)	C15—H15	0.95 (2)
O2—C12	1.2305 (16)	C16—C17	1.365 (3)
C3—C4	1.509 (2)	C16—H16	0.94 (2)
C3—H3A	0.953 (18)	C17—C18	1.387 (3)
C3—H3B	1.010 (18)	C17—H17	0.95 (2)
C5—C6	1.386 (2)	C18—H18	0.97 (2)
C5—C11	1.387 (2)	O3—C19	1.391 (2)
C6—C7	1.388 (2)	O3—H3O	0.84 (3)
C6—H6	0.970 (17)	C19—H19A	0.9600
C7—C8	1.386 (2)	C19—H19B	0.9600
C7—H7	0.954 (19)	C19—H19C	0.9600
C8—C10	1.388 (2)		
N1—C1—C13	109.70 (10)	C8—C9—H9B	109.5
N1—C1—C2	101.20 (10)	H9A—C9—H9B	109.5
C13—C1—C2	115.94 (11)	C8—C9—H9C	109.5
N1—C1—C12	110.13 (10)	H9A—C9—H9C	109.5
C13—C1—C12	113.94 (11)	H9B—C9—H9C	109.5
C2—C1—C12	105.12 (11)	C11—C10—C8	121.32 (15)
C4—N1—C5	123.02 (11)	C11—C10—H10	117.6 (11)
C4—N1—C1	113.58 (11)	C8—C10—H10	121.0 (10)
C5—N1—C1	123.36 (11)	C10—C11—C5	119.88 (14)
C3—C2—C1	103.77 (11)	C10—C11—H11	121.0 (10)
C3—C2—H2A	109.7 (10)	C5—C11—H11	119.0 (10)
C1—C2—H2A	109.2 (10)	O2—C12—N2	122.78 (13)
C3—C2—H2B	113.0 (10)	O2—C12—C1	121.09 (12)
C1—C2—H2B	111.5 (10)	N2—C12—C1	115.95 (12)
H2A—C2—H2B	109.5 (14)	C18—C13—C14	117.86 (15)
C12—N2—H2NA	119.4 (12)	C18—C13—C1	121.16 (14)
C12—N2—H2NB	122.6 (11)	C14—C13—C1	120.78 (13)
H2NA—N2—H2NB	117.0 (17)	C15—C14—C13	121.18 (17)
C4—C3—C2	103.93 (12)	C15—C14—H14	120.1 (12)
C4—C3—H3A	110.7 (11)	C13—C14—H14	118.7 (12)
C2—C3—H3A	113.8 (11)	C16—C15—C14	120.00 (19)
C4—C3—H3B	107.2 (10)	C16—C15—H15	120.7 (13)
C2—C3—H3B	111.2 (10)	C14—C15—H15	119.3 (13)
H3A—C3—H3B	109.6 (15)	C17—C16—C15	119.35 (18)
O1—C4—N1	125.23 (13)	C17—C16—H16	120.4 (13)
O1—C4—C3	126.77 (13)	C15—C16—H16	120.2 (13)
N1—C4—C3	107.99 (12)	C16—C17—C18	121.15 (19)
C6—C5—C11	119.85 (13)	C16—C17—H17	122.0 (15)
C6—C5—N1	119.09 (12)	C18—C17—H17	116.8 (15)
C11—C5—N1	121.06 (12)	C13—C18—C17	120.46 (19)

C5—C6—C7	119.35 (14)	C13—C18—H18	119.8 (12)
C5—C6—H6	118.8 (10)	C17—C18—H18	119.6 (12)
C7—C6—H6	121.8 (10)	C19—O3—H3O	108.3 (17)
C8—C7—C6	121.63 (15)	O3—C19—H19A	109.5
C8—C7—H7	118.1 (11)	O3—C19—H19B	109.5
C6—C7—H7	120.2 (11)	H19A—C19—H19B	109.5
C7—C8—C10	117.95 (14)	O3—C19—H19C	109.5
C7—C8—C9	121.19 (16)	H19A—C19—H19C	109.5
C10—C8—C9	120.85 (16)	H19B—C19—H19C	109.5
C8—C9—H9A	109.5		
C13—C1—N1—C4	142.23 (12)	C7—C8—C10—C11	0.2 (2)
C2—C1—N1—C4	19.24 (14)	C9—C8—C10—C11	−179.83 (15)
C12—C1—N1—C4	−91.60 (13)	C8—C10—C11—C5	0.6 (2)
C13—C1—N1—C5	−40.05 (16)	C6—C5—C11—C10	−0.5 (2)
C2—C1—N1—C5	−163.05 (12)	N1—C5—C11—C10	179.43 (13)
C12—C1—N1—C5	86.11 (15)	N1—C1—C12—O2	15.40 (18)
N1—C1—C2—C3	−29.06 (13)	C13—C1—C12—O2	139.14 (13)
C13—C1—C2—C3	−147.64 (12)	C2—C1—C12—O2	−92.85 (15)
C12—C1—C2—C3	85.58 (13)	N1—C1—C12—N2	−169.31 (12)
C1—C2—C3—C4	29.29 (14)	C13—C1—C12—N2	−45.57 (16)
C5—N1—C4—O1	0.5 (2)	C2—C1—C12—N2	82.44 (14)
C1—N1—C4—O1	178.18 (13)	N1—C1—C13—C18	−84.59 (16)
C5—N1—C4—C3	−178.68 (12)	C2—C1—C13—C18	29.21 (19)
C1—N1—C4—C3	−0.96 (15)	C12—C1—C13—C18	151.44 (14)
C2—C3—C4—O1	162.53 (14)	N1—C1—C13—C14	90.18 (15)
C2—C3—C4—N1	−18.35 (15)	C2—C1—C13—C14	−156.02 (13)
C4—N1—C5—C6	−76.02 (17)	C12—C1—C13—C14	−33.79 (17)
C1—N1—C5—C6	106.48 (15)	C18—C13—C14—C15	−0.6 (2)
C4—N1—C5—C11	104.04 (15)	C1—C13—C14—C15	−175.51 (14)
C1—N1—C5—C11	−73.46 (17)	C13—C14—C15—C16	−0.3 (3)
C11—C5—C6—C7	−0.4 (2)	C14—C15—C16—C17	0.9 (3)
N1—C5—C6—C7	179.62 (13)	C15—C16—C17—C18	−0.6 (3)
C5—C6—C7—C8	1.3 (2)	C14—C13—C18—C17	0.9 (3)
C6—C7—C8—C10	−1.2 (2)	C1—C13—C18—C17	175.77 (16)
C6—C7—C8—C9	178.85 (15)	C16—C17—C18—C13	−0.3 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3o···O2	0.84 (2)	1.90 (2)	2.741 (2)	176 (2)
N2^{i}—H2nB^{i}···O3	0.91 (2)	2.00 (2)	2.860 (2)	156 (2)

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

Fig. 1

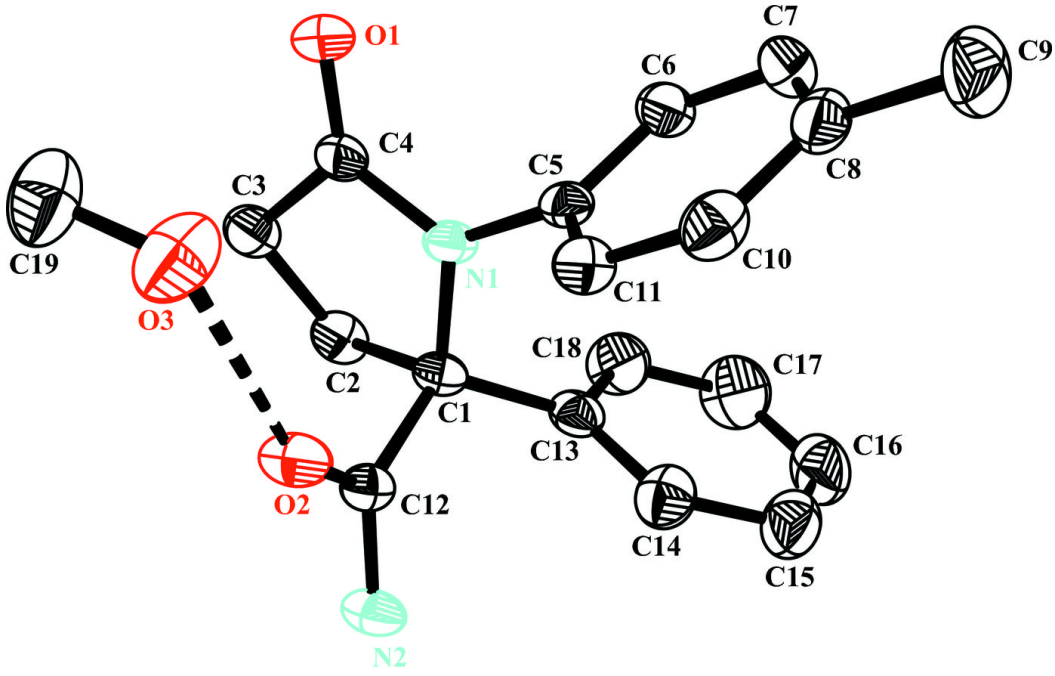
O1
C7
C9
C6
C4
C5
C8
C3
C19
N1
C10
O3
C11
C18
C17
C2
C1
C16
C13
O2
C12
C14
C15
N2

Fig. 2