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(*R*)-Methyl 2-(furan-2-carboxamido)-4-methylpentanoate

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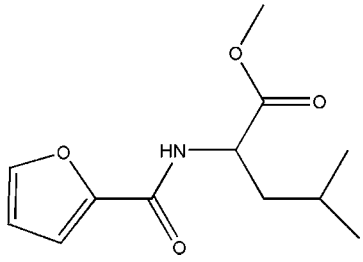
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; R factor = 0.049; wR factor = 0.134; data-to-parameter ratio = 10.1.

The title compound, $C_{12}H_{17}NO_4$, was synthesized by the condensation reaction of L-leucine methyl ester with furan-2-carbonyl chloride at room temperature. There are two molecules in the asymmetric unit. All bond lengths and angles are within normal ranges. Intermolecular N—H···O interactions link the molecules to form one-dimensional polymeric chains along the *c* axis.

Related literature

For related literature, see: El-Naggar *et al.* (1976); Gomis-Ruth *et al.* (1998); Wipf & Halter (2005); Zeng & Liu (2005).



Experimental

Crystal data

$C_{12}H_{17}NO_4$
M_r = 239.27
Orthorhombic, $P2_12_12_1$
a = 8.7674 (10) Å
b = 16.1703 (18) Å
c = 18.224 (2) Å
V = 2583.6 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 (2) K
0.50 × 0.40 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.957, T_{max} = 0.982
13310 measured reflections
3189 independent reflections
2685 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.134
S = 1.05
3189 reflections
315 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O6^{i}	0.88	2.16	2.994 (3)	159
N2—H2···O2	0.88	2.00	2.847 (3)	162
N2—H2···O5	0.83	2.42	2.751 (4)	105

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2093).

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supplementary materials

Acta Cryst. (2007). E**63**, o3644 [**doi:10.1107/S1600536807036410**]

(*R*)-Methyl 2-(furan-2-carboxamido)-4-methylpentanoate

W.-J. Xu, X.-J. Liao, S.-H. Xu and P.-R. Liu

Comment

Furan derivatives are well known in many organisms (Wipf *et al.*, 2005), and some of them are bioactive substances (Gomis-Ruth *et al.*, 1998). In our search for bioactive compounds, a series of furan(2-carbonyl)amino acid esters, including the title compound, (I), have been synthesized by the reaction of amino acid esters with Furan-2-carbonyl chloride. We report here its crystal structure. Bond lengths and angles are unexceptional and are in good agreement with the corresponding values in (*S*)-Methyl 4-methyl-2-(1*H*-pyrrole-2-carboxamido)-pentanoate (Zeng & Liu, 2005) and 1-(4-methoxyphenyl)-3-(3-methyl-2-furan-carbonyl)-thiourea (Hritzova *et al.*, 2005). There are two molecules in the asymmetric unit (Fig. 1) and only one kind of intermolecular hydrogen bonds in the crystal structure. Every molecule is connected with two other molecules by hydrogen-bond interactions, generating extended chains along the *c* axis, Figure 2.

Experimental

The synthesis of (I) was reported by El-Naggar *et al.*,1976. A solution of Furan-2-carbonyl chloride (0.66 g, 5 mmol) in dichloromethane (2.5 ml) was added dropwise, under stirring, to *L*-leucine methyl ester (0.91 g, 5 mmol) in dichloromethane (5 ml). The mixture was stirred at room temperature for 2 h and then poured into water. After filtration, the solution was wash with water(5 ml), The organic phase was dried over Na_2SO_4 and evaporated under reduced pressure. The residue was dissolved in ethanol at room temperature. Colorless orthorhombic crystals suitable for X-ray analysis (m.p. 362 K, 81.6 percent yield) grew over a period of one week when the solution was exposed to air.

Refinement

Hydrogen atoms attached to C or N atoms were located at geometrically calculated positions [0.95 (CH), 0.99 (CH_2), 0.98 (CH_3), 0.88 (NH)] and refined with isotropic thermal parameters U_{iso}(H) equal to 1.2 for CH_2, CH, and NH, 1.5 for CH_3 U_{eq}(C atoms). The highest positive and negative electron-density residuals are located 0.93 and 0.84Å from C14 and C23 respectively.

Figures

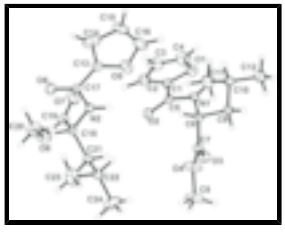

Fig. 1. The molecular structure of the title compound.

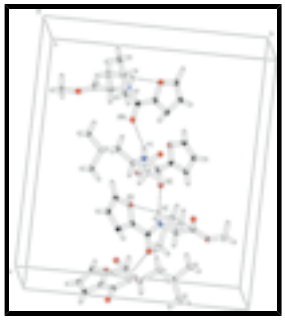

Fig. 2. The crystal structure of (I), viewed along the *a* axis. Dashed lines show N—H···O interactions. [Symmetry code: (i) −*x* + 1/2, −*y* + 1, *z* − 1/2]

(*R*)-Methyl 2-(furan-2-carboxamido)-4-methylpentanoate

Crystal data

$C_{12}H_{17}NO_4$	D_x = 1.230 Mg m^{-3}
M_r = 239.27	Mo *K*α radiation λ = 0.71073 Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 13310 reflections
a = 8.7674 (10) Å	θ = 12–18º
b = 16.1703 (18) Å	μ = 0.09 mm^{-1}
c = 18.224 (2) Å	*T* = 173 (2) K
V = 2583.6 (5) Å^3	Block, colourless
Z = 8	0.50 × 0.40 × 0.20 mm
F_{000} = 1024	

Data collection

Bruker SMART 1000 CCD aea-detector diffractometer	3189 independent reflections
Radiation source: fine-focus sealed tube	2685 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
T = 293(2) K	θ_{max} = 27.1º
ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −9→11
T_{min} = 0.957, T_{max} = 0.982	*k* = −13→20
13310 measured reflections	*l* = −23→22

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 1.1602P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.049	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.134	$\Delta\rho_{max}$ = 0.67 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −0.21 e Å^{-3}

3189 reflections

315 parameters

3 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0046 (9)

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}
O1	0.1237 (3)	0.61581 (14)	0.45097 (12)	0.0445 (5)
O2	0.4018 (3)	0.58090 (14)	0.58910 (11)	0.0404 (5)
O3	0.6183 (3)	0.55287 (14)	0.44903 (13)	0.0461 (6)
O4	0.7289 (3)	0.45796 (17)	0.52091 (19)	0.0665 (9)
O5	0.2261 (3)	0.46393 (17)	0.69428 (15)	0.0632 (8)
O6	0.3297 (3)	0.56474 (14)	0.86200 (11)	0.0434 (5)
O7	0.2604 (3)	0.74834 (16)	0.72373 (15)	0.0574 (7)
O8	0.4538 (3)	0.81196 (13)	0.78045 (15)	0.0531 (7)
N1	0.3328 (3)	0.49843 (15)	0.49519 (14)	0.0319 (5)
H1	0.2638	0.4855	0.4621	0.038*
N2	0.3946 (3)	0.59578 (14)	0.74474 (13)	0.0328 (5)
H2	0.3900	0.5799	0.6986	0.039*
C1	0.2009 (3)	0.62688 (18)	0.51507 (16)	0.0336 (6)
C2	0.1566 (4)	0.6981 (2)	0.5477 (2)	0.0490 (8)
H2A	0.1927	0.7201	0.5928	0.059*
C3	0.0452 (5)	0.7331 (2)	0.5007 (3)	0.0592 (10)
H3	−0.0078	0.7837	0.5080	0.071*
C4	0.0290 (5)	0.6822 (2)	0.4449 (2)	0.0573 (10)
H4	−0.0400	0.6907	0.4054	0.069*
C5	0.3179 (3)	0.56685 (18)	0.53628 (14)	0.0305 (6)
C6	0.4648 (3)	0.44653 (18)	0.50666 (16)	0.0332 (6)
H6	0.4681	0.4293	0.5593	0.040*
C7	0.6099 (4)	0.49425 (19)	0.48859 (18)	0.0382 (7)
C8	0.8780 (5)	0.4917 (3)	0.5032 (3)	0.0790 (15)

H8A	0.8984	0.4840	0.4508	0.118*
H8B	0.9563	0.4630	0.5319	0.118*
H8C	0.8799	0.5508	0.5149	0.118*
C9	0.4580 (3)	0.36901 (17)	0.45842 (17)	0.0345 (6)
H9A	0.4396	0.3865	0.4071	0.041*
H9B	0.5590	0.3417	0.4599	0.041*
C10	0.3368 (4)	0.30551 (18)	0.47946 (16)	0.0359 (7)
H10	0.2353	0.3337	0.4812	0.043*
C11	0.3688 (5)	0.2675 (2)	0.5542 (2)	0.0537 (9)
H11A	0.2890	0.2271	0.5660	0.081*
H11B	0.3699	0.3110	0.5916	0.081*
H11C	0.4681	0.2397	0.5532	0.081*
C12	0.3321 (5)	0.2390 (2)	0.4208 (2)	0.0516 (9)
H12A	0.3141	0.2645	0.3728	0.077*
H12B	0.2495	0.2000	0.4317	0.077*
H12C	0.4296	0.2093	0.4200	0.077*
C13	0.2279 (3)	0.48155 (17)	0.76822 (17)	0.0346 (6)
C14	0.1322 (5)	0.4294 (3)	0.8043 (2)	0.0664 (12)
H14	0.1096	0.4271	0.8552	0.080*
C15	0.0722 (4)	0.3773 (2)	0.7445 (3)	0.0614 (11)
H15	0.0015	0.3333	0.7503	0.074*
C16	0.1313 (5)	0.4012 (3)	0.6822 (3)	0.0745 (13)
H16	0.1100	0.3776	0.6356	0.089*
C17	0.3217 (3)	0.55087 (17)	0.79574 (15)	0.0314 (6)
C18	0.4802 (3)	0.66905 (16)	0.76288 (15)	0.0308 (6)
H18	0.5107	0.6656	0.8157	0.037*
C19	0.3825 (4)	0.74590 (18)	0.75269 (16)	0.0362 (6)
C20	0.3752 (5)	0.8901 (2)	0.7729 (3)	0.0628 (11)
H20A	0.3565	0.9013	0.7208	0.094*
H20B	0.4381	0.9344	0.7936	0.094*
H20C	0.2777	0.8876	0.7991	0.094*
C21	0.6249 (4)	0.67787 (17)	0.71650 (17)	0.0355 (6)
H21A	0.5948	0.6845	0.6645	0.043*
H21B	0.6784	0.7291	0.7315	0.043*
C22	0.7360 (4)	0.60601 (19)	0.72204 (19)	0.0413 (7)
H22	0.6845	0.5562	0.7010	0.050*
C23	0.7791 (6)	0.5861 (3)	0.7997 (2)	0.0776 (15)
H23A	0.8320	0.6335	0.8215	0.116*
H23B	0.8467	0.5378	0.8002	0.116*
H23C	0.6869	0.5739	0.8281	0.116*
C24	0.8755 (5)	0.6246 (3)	0.6743 (3)	0.0844 (16)
H24A	0.8422	0.6378	0.6243	0.127*
H24B	0.9424	0.5761	0.6732	0.127*
H24C	0.9310	0.6718	0.6948	0.127*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

O1	0.0484 (13)	0.0439 (12)	0.0411 (12)	0.0026 (11)	−0.0065 (11)	0.0066 (10)
O2	0.0405 (12)	0.0506 (13)	0.0300 (10)	0.0006 (11)	−0.0022 (9)	−0.0072 (9)
O3	0.0451 (13)	0.0420 (12)	0.0511 (13)	−0.0068 (11)	0.0038 (11)	0.0067 (11)
O4	0.0329 (12)	0.0489 (14)	0.118 (2)	−0.0080 (12)	−0.0183 (15)	0.0253 (16)
O5	0.0635 (17)	0.0629 (16)	0.0634 (16)	−0.0149 (15)	−0.0060 (14)	−0.0204 (14)
O6	0.0537 (13)	0.0434 (12)	0.0330 (11)	−0.0086 (11)	0.0053 (10)	0.0030 (10)
O7	0.0539 (15)	0.0556 (14)	0.0627 (15)	0.0180 (13)	−0.0205 (13)	−0.0142 (13)
O8	0.0473 (14)	0.0269 (11)	0.0851 (18)	0.0032 (10)	−0.0039 (13)	−0.0033 (11)
N1	0.0307 (12)	0.0323 (12)	0.0326 (12)	0.0003 (10)	−0.0055 (11)	−0.0018 (10)
N2	0.0396 (13)	0.0315 (12)	0.0275 (11)	−0.0055 (11)	0.0016 (11)	−0.0014 (9)
C1	0.0308 (15)	0.0336 (14)	0.0364 (15)	−0.0043 (12)	0.0052 (12)	0.0009 (12)
C2	0.0434 (18)	0.0398 (17)	0.064 (2)	−0.0004 (15)	0.0038 (17)	−0.0098 (16)
C3	0.050 (2)	0.0391 (19)	0.088 (3)	0.0081 (16)	0.001 (2)	0.005 (2)
C4	0.056 (2)	0.052 (2)	0.064 (2)	0.0095 (19)	−0.009 (2)	0.0203 (19)
C5	0.0282 (13)	0.0360 (14)	0.0272 (13)	−0.0068 (12)	0.0046 (11)	−0.0013 (11)
C6	0.0302 (14)	0.0325 (14)	0.0370 (14)	−0.0032 (12)	−0.0031 (12)	0.0015 (13)
C7	0.0349 (15)	0.0322 (15)	0.0474 (18)	−0.0032 (13)	−0.0032 (15)	−0.0024 (13)
C8	0.036 (2)	0.067 (3)	0.134 (4)	−0.012 (2)	−0.009 (3)	0.008 (3)
C9	0.0315 (14)	0.0312 (14)	0.0409 (16)	−0.0003 (12)	0.0053 (13)	0.0010 (13)
C10	0.0330 (15)	0.0303 (14)	0.0443 (16)	−0.0028 (13)	0.0009 (13)	0.0020 (12)
C11	0.056 (2)	0.055 (2)	0.0502 (19)	−0.0210 (19)	−0.0034 (18)	0.0124 (17)
C12	0.061 (2)	0.0374 (17)	0.056 (2)	−0.0111 (17)	0.0045 (18)	−0.0041 (16)
C13	0.0312 (14)	0.0315 (14)	0.0410 (16)	0.0014 (12)	0.0004 (13)	0.0043 (12)
C14	0.046 (2)	0.070 (3)	0.084 (3)	0.0039 (19)	0.006 (2)	0.039 (2)
C15	0.0416 (19)	0.0365 (18)	0.106 (3)	−0.0111 (16)	−0.013 (2)	−0.001 (2)
C16	0.066 (3)	0.062 (3)	0.095 (3)	−0.019 (2)	−0.010 (3)	−0.020 (3)
C17	0.0326 (14)	0.0294 (13)	0.0322 (14)	0.0040 (12)	0.0036 (12)	0.0036 (12)
C18	0.0375 (15)	0.0261 (13)	0.0288 (13)	−0.0025 (12)	−0.0011 (12)	0.0007 (11)
C19	0.0389 (15)	0.0344 (15)	0.0352 (14)	0.0021 (13)	0.0013 (14)	0.0018 (12)
C20	0.066 (3)	0.0301 (16)	0.092 (3)	0.0137 (17)	0.007 (2)	0.0027 (18)
C21	0.0403 (16)	0.0269 (13)	0.0394 (15)	−0.0041 (12)	0.0001 (13)	−0.0010 (12)
C22	0.0374 (16)	0.0318 (14)	0.0548 (19)	0.0011 (13)	0.0017 (15)	−0.0077 (14)
C23	0.077 (3)	0.083 (3)	0.073 (3)	0.045 (3)	−0.029 (2)	−0.012 (2)
C24	0.059 (3)	0.067 (3)	0.127 (4)	0.006 (2)	0.041 (3)	−0.010 (3)

Geometric parameters (Å, °)

O1—C1	1.362 (4)	C10—C12	1.517 (4)
O1—C4	1.362 (4)	C10—C11	1.521 (4)
O2—C5	1.233 (3)	C10—H10	1.0000
O3—C7	1.193 (4)	C11—H11A	0.9800
O4—C7	1.335 (4)	C11—H11B	0.9800
O4—C8	1.453 (5)	C11—H11C	0.9800
O5—C16	1.329 (5)	C12—H12A	0.9800
O5—C13	1.377 (4)	C12—H12B	0.9800
O6—C17	1.230 (3)	C12—H12C	0.9800
O7—C19	1.194 (4)	C13—C14	1.359 (5)
O8—C19	1.337 (4)	C13—C17	1.478 (4)
O8—C20	1.446 (4)	C14—C15	1.474 (5)

N1—C5	1.342 (4)	C14—H14	0.9500
N1—C6	1.444 (4)	C15—C16	1.307 (6)
N1—H1	0.8800	C15—H15	0.9500
N2—C17	1.342 (4)	C16—H16	0.9500
N2—C18	1.441 (4)	C18—C19	1.520 (4)
N2—H2	0.8800	C18—C21	1.531 (4)
C1—C2	1.353 (4)	C18—H18	1.0000
C1—C5	1.465 (4)	C20—H20A	0.9800
C2—C3	1.417 (6)	C20—H20B	0.9800
C2—H2A	0.9500	C20—H20C	0.9800
C3—C4	1.315 (6)	C21—C22	1.520 (4)
C3—H3	0.9500	C21—H21A	0.9900
C4—H4	0.9500	C21—H21B	0.9900
C6—C7	1.524 (4)	C22—C23	1.499 (5)
C6—C9	1.532 (4)	C22—C24	1.530 (5)
C6—H6	1.0000	C22—H22	1.0000
C8—H8A	0.9800	C23—H23A	0.9800
C8—H8B	0.9800	C23—H23B	0.9800
C8—H8C	0.9800	C23—H23C	0.9800
C9—C10	1.527 (4)	C24—H24A	0.9800
C9—H9A	0.9900	C24—H24B	0.9800
C9—H9B	0.9900	C24—H24C	0.9800
C1—O1—C4	105.6 (3)	C10—C12—H12B	109.5
C7—O4—C8	116.2 (3)	H12A—C12—H12B	109.5
C16—O5—C13	109.1 (3)	C10—C12—H12C	109.5
C19—O8—C20	116.1 (3)	H12A—C12—H12C	109.5
C5—N1—C6	118.4 (2)	H12B—C12—H12C	109.5
C5—N1—H1	120.8	C14—C13—O5	109.7 (3)
C6—N1—H1	120.8	C14—C13—C17	130.5 (3)
C17—N2—C18	122.3 (2)	O5—C13—C17	119.7 (3)
C17—N2—H2	118.9	C13—C14—C15	102.5 (3)
C18—N2—H2	118.9	C13—C14—H14	128.7
C2—C1—O1	110.3 (3)	C15—C14—H14	128.7
C2—C1—C5	130.5 (3)	C16—C15—C14	109.4 (3)
O1—C1—C5	119.2 (3)	C16—C15—H15	125.3
C1—C2—C3	105.8 (3)	C14—C15—H15	125.3
C1—C2—H2A	127.1	C15—C16—O5	109.2 (4)
C3—C2—H2A	127.1	C15—C16—H16	125.4
C4—C3—C2	107.0 (3)	O5—C16—H16	125.4
C4—C3—H3	126.5	O6—C17—N2	123.6 (3)
C2—C3—H3	126.5	O6—C17—C13	120.2 (3)
C3—C4—O1	111.4 (3)	N2—C17—C13	116.1 (2)
C3—C4—H4	124.3	N2—C18—C19	110.5 (2)
O1—C4—H4	124.3	N2—C18—C21	112.4 (2)
O2—C5—N1	122.0 (3)	C19—C18—C21	108.8 (2)
O2—C5—C1	120.1 (3)	N2—C18—H18	108.3
N1—C5—C1	117.9 (2)	C19—C18—H18	108.3
N1—C6—C7	110.1 (2)	C21—C18—H18	108.3
N1—C6—C9	111.2 (2)	O7—C19—O8	124.0 (3)

C7—C6—C9	108.8 (2)	O7—C19—C18	125.9 (3)
N1—C6—H6	108.9	O8—C19—C18	110.1 (2)
C7—C6—H6	108.9	O8—C20—H20A	109.5
C9—C6—H6	108.9	O8—C20—H20B	109.5
O3—C7—O4	124.6 (3)	H20A—C20—H20B	109.5
O3—C7—C6	125.8 (3)	O8—C20—H20C	109.5
O4—C7—C6	109.6 (2)	H20A—C20—H20C	109.5
O4—C8—H8A	109.5	H20B—C20—H20C	109.5
O4—C8—H8B	109.5	C22—C21—C18	115.0 (2)
H8A—C8—H8B	109.5	C22—C21—H21A	108.5
O4—C8—H8C	109.5	C18—C21—H21A	108.5
H8A—C8—H8C	109.5	C22—C21—H21B	108.5
H8B—C8—H8C	109.5	C18—C21—H21B	108.5
C10—C9—C6	115.7 (2)	H21A—C21—H21B	107.5
C10—C9—H9A	108.4	C23—C22—C21	112.9 (3)
C6—C9—H9A	108.4	C23—C22—C24	112.2 (4)
C10—C9—H9B	108.4	C21—C22—C24	108.9 (3)
C6—C9—H9B	108.4	C23—C22—H22	107.6
H9A—C9—H9B	107.4	C21—C22—H22	107.6
C12—C10—C11	110.4 (3)	C24—C22—H22	107.6
C12—C10—C9	108.6 (3)	C22—C23—H23A	109.5
C11—C10—C9	111.6 (3)	C22—C23—H23B	109.5
C12—C10—H10	108.7	H23A—C23—H23B	109.5
C11—C10—H10	108.7	C22—C23—H23C	109.5
C9—C10—H10	108.7	H23A—C23—H23C	109.5
C10—C11—H11A	109.5	H23B—C23—H23C	109.5
C10—C11—H11B	109.5	C22—C24—H24A	109.5
H11A—C11—H11B	109.5	C22—C24—H24B	109.5
C10—C11—H11C	109.5	H24A—C24—H24B	109.5
H11A—C11—H11C	109.5	C22—C24—H24C	109.5
H11B—C11—H11C	109.5	H24A—C24—H24C	109.5
C10—C12—H12A	109.5	H24B—C24—H24C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O6^{i}	0.88	2.16	2.994 (3)	159
N2—H2···O2	0.88	2.00	2.847 (3)	162
N2—H2···O5	0.83	2.42	2.751 (4)	105

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

Fig. 1

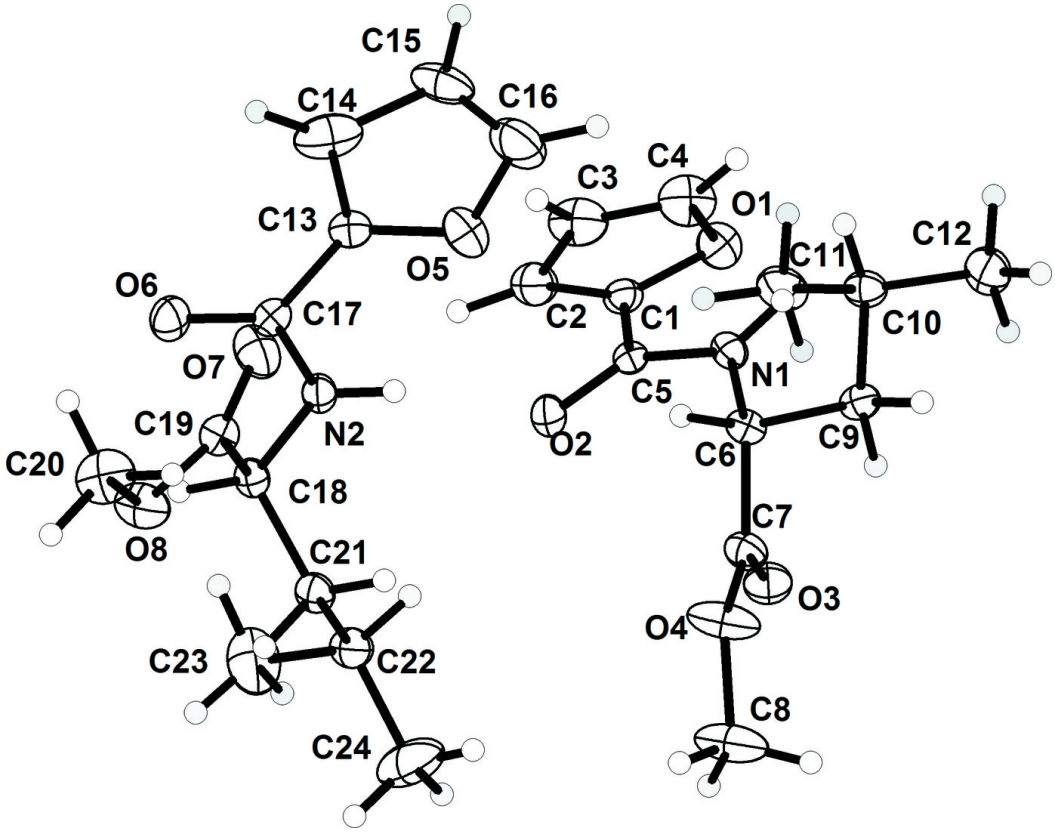
C15
C14
C16
C4
C3
O1
C13
O5
C12
C11
O6
C17
C2
C1
C10
O7
N1
C5
C19
N2
C9
O2
C6
C20
C18
C7
O8
C21
O3
O4
C23
C22
C8
C24

Fig. 2