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Ethyl 2-[(*Z*)-4-isobutyl-5-oxo-2-(phenylimino)imidazolidin-1-yl]acetate

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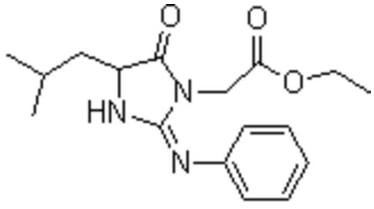
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; R factor = 0.069; wR factor = 0.195; data-to-parameter ratio = 14.7.

In the crystal structure of the title compound, $C_{17}H_{23}N_3O_3$, intermolecular N—H···O and C—H···O hydrogen bonds are present. The planar heterocyclic ring makes a dihedral angle of 64.4 (1)° with the phenyl ring.

Related literature

Related preparation and biological activity is described by Lacroix *et al.* (2000*a*,*b*). For related literature, see: Li & Hu (2006).



Experimental

Crystal data

$C_{17}H_{23}N_3O_3$
M_r = 317.38
Orthorhombic, *Pbca*
a = 16.059 (2) Å
b = 10.6310 (16) Å
c = 20.690 (3) Å
V = 3532.2 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 292 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.984, T_{max} = 0.992
26346 measured reflections
3097 independent reflections
2154 reflections with $I > 2\sigma(I)$
R_{int} = 0.101

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.195
S = 1.06
3097 reflections
211 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O2^{i}	0.93	2.47	3.257 (4)	143
N2—H2A···O1^{i}	0.86	2.31	3.137 (3)	162

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2473).

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supplementary materials

Acta Cryst. (2007). E**63**, o4768 [**doi:10.1107/S1600536807058473**]

Ethyl 2-[(*Z*)-4-isobutyl-5-oxo-2-(phenylimino)imidazolidin-1-yl]acetate

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Refinement

All H atoms were located in difference maps and treated as riding atoms, except those at N1, with the following distance restraints: C—H = 0.93 Å, U_{iso}=1.2U_{eq} (C) for Csp^2, C—H = 0.98 Å, U_{iso} = 1.2U_{eq} (C) for CH, C—H = 0.97 Å, U_{iso} = 1.2U_{eq} (C) for CH_2, N—H = 0.86 Å, U_{iso} = 1.2U_{eq} (N) for NH, C—H = 0.96 Å, U_{iso} = 1.5U_{eq} (C) for CH_3.

Figures

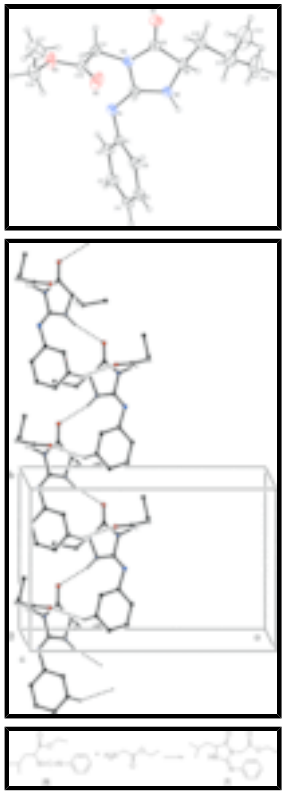

Fig. 1. The molecular structure of the title compound, showing the atom-labeling scheme.
Fig. 2. The packing in the crystal structure, showing the N—H···O and C—H···O hydrogen bonds as dashed lines.

Ethyl 2-[(*Z*)-4-isobutyl-5-oxo-2-(phenylimino)imidazolidin-1-yl]acetate

Crystal data

$C_{17}H_{23}N_3O_3$	F_{000} = 1360
M_r = 317.38	D_x = 1.194 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3517 reflections

a = 16.059 (2) Å	θ = 2.3–21.8º
b = 10.6310 (16) Å	μ = 0.08 mm^{-1}
c = 20.690 (3) Å	T = 292 (2) K
V = 3532.2 (9) $Å^3$	Block, colorless
Z = 8	0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer	3097 independent reflections
Radiation source: fine-focus sealed tube	2154 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.101
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$h = -19 \rightarrow 19$
T_{min} = 0.984, T_{max} = 0.992	$k = -12 \rightarrow 12$
26346 measured reflections	$l = -24 \rightarrow 24$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.069	H-atom parameters constrained
$wR(F^2)$ = 0.195	$w = 1/[\sigma^2(F_o^2) + (0.0923P)^2 + 1.1347P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.002
3097 reflections	$\Delta\rho_{max}$ = 0.34 e $Å^{-3}$
211 parameters	$\Delta\rho_{min}$ = −0.18 e $Å^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.09982 (18)	0.7576 (3)	0.08787 (13)	0.0458 (7)
C2	0.0456 (2)	0.6621 (3)	0.06955 (14)	0.0551 (8)
H2	−0.0046	0.6822	0.0496	0.066*
C3	0.0655 (2)	0.5376 (3)	0.08081 (17)	0.0659 (9)
H3	0.0290	0.4745	0.0679	0.079*
C4	0.1392 (2)	0.5062 (3)	0.11101 (15)	0.0603 (9)
H4	0.1525	0.4223	0.1184	0.072*
C5	0.19213 (19)	0.5989 (3)	0.12982 (15)	0.0591 (9)
H5	0.2415	0.5782	0.1508	0.071*
C6	0.17313 (18)	0.7238 (3)	0.11799 (14)	0.0547 (8)
H6	0.2105	0.7861	0.1306	0.066*
C7	0.11827 (17)	0.9583 (3)	0.04646 (12)	0.0424 (7)
C9	0.15621 (18)	1.1546 (3)	0.00999 (13)	0.0479 (7)
C10	0.2068 (2)	1.0674 (3)	−0.09344 (15)	0.0645 (9)
H10A	0.1498	1.0486	−0.1056	0.077*
H10B	0.2182	1.1534	−0.1065	0.077*
C11	0.2631 (3)	0.9824 (5)	−0.13001 (18)	0.0954 (14)
H11	0.2525	0.8962	−0.1153	0.114*
C12	0.3534 (3)	1.0105 (7)	−0.1188 (3)	0.162 (3)
H12A	0.3643	1.0971	−0.1287	0.244*
H12B	0.3868	0.9577	−0.1462	0.244*
H12C	0.3671	0.9944	−0.0744	0.244*
C13	0.2439 (4)	0.9881 (8)	−0.2014 (2)	0.167 (3)
H13A	0.1864	0.9671	−0.2084	0.251*
H13B	0.2786	0.9293	−0.2241	0.251*
H13C	0.2544	1.0716	−0.2172	0.251*
C14	0.02954 (18)	1.1411 (3)	0.07902 (14)	0.0508 (8)
H14A	−0.0183	1.0858	0.0756	0.061*
H14B	0.0147	1.2210	0.0595	0.061*
C15	0.04940 (19)	1.1616 (3)	0.14927 (14)	0.0503 (7)
C16	−0.0116 (3)	1.2182 (4)	0.24988 (18)	0.0879 (13)
H16A	−0.0635	1.1980	0.2714	0.106*
H16B	0.0318	1.1664	0.2687	0.106*
C17	0.0080 (4)	1.3489 (5)	0.2607 (2)	0.1209 (18)
H17A	0.0605	1.3684	0.2409	0.181*
H17B	0.0112	1.3648	0.3063	0.181*
H17C	−0.0347	1.4005	0.2420	0.181*
N1	0.07527 (15)	0.8841 (2)	0.08053 (12)	0.0518 (6)
N2	0.18427 (15)	0.9414 (2)	0.00589 (11)	0.0501 (6)
H2A	0.2208	0.8838	0.0119	0.060*
C8	0.21386 (19)	1.0593 (3)	−0.02093 (13)	0.0492 (7)
H8	0.2715	1.0748	−0.0074	0.059*
N3	0.09884 (14)	1.0867 (2)	0.04362 (11)	0.0444 (6)
O1	0.15797 (13)	1.2674 (2)	0.00413 (11)	0.0635 (6)
O2	0.11634 (16)	1.1560 (3)	0.17248 (12)	0.0920 (9)

O3	−0.01909 (14)	1.1890 (2)	0.18119 (10)	0.0732 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0515 (17)	0.0453 (17)	0.0406 (15)	−0.0024 (14)	0.0101 (13)	0.0044 (12)
C2	0.0557 (18)	0.054 (2)	0.0560 (19)	−0.0059 (15)	−0.0061 (14)	0.0081 (14)
C3	0.068 (2)	0.049 (2)	0.081 (2)	−0.0111 (17)	−0.0014 (18)	0.0035 (17)
C4	0.066 (2)	0.049 (2)	0.066 (2)	0.0048 (16)	0.0110 (17)	0.0138 (15)
C5	0.0473 (18)	0.067 (2)	0.064 (2)	0.0020 (16)	0.0024 (15)	0.0149 (16)
C6	0.0526 (18)	0.058 (2)	0.0531 (18)	−0.0125 (15)	0.0022 (14)	0.0054 (14)
C7	0.0502 (16)	0.0414 (17)	0.0357 (14)	−0.0016 (13)	0.0013 (12)	−0.0010 (12)
C9	0.0526 (17)	0.0422 (18)	0.0489 (16)	−0.0031 (14)	−0.0012 (13)	0.0044 (13)
C10	0.065 (2)	0.075 (2)	0.0532 (19)	−0.0010 (18)	0.0023 (16)	0.0055 (16)
C11	0.104 (3)	0.123 (4)	0.059 (2)	0.020 (3)	0.009 (2)	−0.007 (2)
C12	0.090 (4)	0.305 (10)	0.091 (3)	0.043 (5)	0.022 (3)	−0.007 (4)
C13	0.157 (5)	0.282 (9)	0.063 (3)	0.058 (5)	0.006 (3)	−0.046 (4)
C14	0.0510 (17)	0.0511 (18)	0.0502 (17)	0.0098 (14)	0.0016 (14)	−0.0031 (13)
C15	0.0499 (18)	0.0472 (18)	0.0538 (18)	0.0065 (14)	0.0047 (15)	0.0007 (13)
C16	0.097 (3)	0.110 (3)	0.057 (2)	−0.003 (2)	0.026 (2)	−0.010 (2)
C17	0.191 (5)	0.101 (4)	0.071 (3)	−0.014 (4)	0.018 (3)	−0.024 (2)
N1	0.0576 (15)	0.0453 (15)	0.0525 (14)	−0.0005 (12)	0.0111 (12)	0.0061 (11)
N2	0.0576 (15)	0.0439 (14)	0.0488 (14)	0.0064 (11)	0.0124 (11)	0.0031 (11)
C8	0.0517 (17)	0.0482 (18)	0.0477 (16)	−0.0010 (14)	0.0101 (13)	0.0053 (13)
N3	0.0521 (14)	0.0361 (13)	0.0449 (13)	0.0010 (11)	0.0068 (11)	−0.0007 (10)
O1	0.0723 (15)	0.0399 (14)	0.0782 (15)	−0.0001 (10)	0.0046 (12)	0.0065 (11)
O2	0.0664 (16)	0.145 (3)	0.0649 (16)	0.0304 (17)	−0.0104 (13)	−0.0237 (15)
O3	0.0633 (15)	0.0986 (19)	0.0576 (14)	0.0068 (13)	0.0157 (11)	−0.0164 (12)

Geometric parameters (Å, °)

C1—C6	1.380 (4)	C11—H11	0.9800
C1—C2	1.391 (4)	C12—H12A	0.9600
C1—N1	1.410 (4)	C12—H12B	0.9600
C2—C3	1.381 (5)	C12—H12C	0.9600
C2—H2	0.9300	C13—H13A	0.9600
C3—C4	1.378 (5)	C13—H13B	0.9600
C3—H3	0.9300	C13—H13C	0.9600
C4—C5	1.358 (5)	C14—N3	1.453 (3)
C4—H4	0.9300	C14—C15	1.504 (4)
C5—C6	1.385 (4)	C14—H14A	0.9700
C5—H5	0.9300	C14—H14B	0.9700
C6—H6	0.9300	C15—O2	1.179 (3)
C7—N1	1.263 (3)	C15—O3	1.316 (3)
C7—N2	1.364 (3)	C16—C17	1.441 (6)
C7—N3	1.401 (3)	C16—O3	1.460 (4)
C9—O1	1.205 (3)	C16—H16A	0.9700
C9—N3	1.362 (4)	C16—H16B	0.9700
C9—C8	1.514 (4)	C17—H17A	0.9600

C10—C11	1.485 (5)	C17—H17B	0.9600
C10—C8	1.507 (4)	C17—H17C	0.9600
C10—H10A	0.9700	N2—C8	1.451 (4)
C10—H10B	0.9700	N2—H2A	0.8573
C11—C12	1.499 (7)	C8—H8	0.9800
C11—C13	1.511 (6)		
C6—C1—C2	117.8 (3)	C11—C13—H13A	109.5
C6—C1—N1	122.4 (3)	C11—C13—H13B	109.5
C2—C1—N1	119.5 (3)	H13A—C13—H13B	109.5
C3—C2—C1	120.6 (3)	C11—C13—H13C	109.5
C3—C2—H2	119.7	H13A—C13—H13C	109.5
C1—C2—H2	119.7	H13B—C13—H13C	109.5
C4—C3—C2	120.5 (3)	N3—C14—C15	112.5 (2)
C4—C3—H3	119.8	N3—C14—H14A	109.1
C2—C3—H3	119.8	C15—C14—H14A	109.1
C5—C4—C3	119.4 (3)	N3—C14—H14B	109.1
C5—C4—H4	120.3	C15—C14—H14B	109.1
C3—C4—H4	120.3	H14A—C14—H14B	107.8
C4—C5—C6	120.5 (3)	O2—C15—O3	124.7 (3)
C4—C5—H5	119.8	O2—C15—C14	125.4 (3)
C6—C5—H5	119.8	O3—C15—C14	109.9 (3)
C1—C6—C5	121.2 (3)	C17—C16—O3	111.9 (3)
C1—C6—H6	119.4	C17—C16—H16A	109.2
C5—C6—H6	119.4	O3—C16—H16A	109.2
N1—C7—N2	133.3 (3)	C17—C16—H16B	109.2
N1—C7—N3	120.6 (2)	O3—C16—H16B	109.2
N2—C7—N3	106.0 (2)	H16A—C16—H16B	107.9
O1—C9—N3	126.5 (3)	C16—C17—H17A	109.5
O1—C9—C8	127.5 (3)	C16—C17—H17B	109.5
N3—C9—C8	105.9 (2)	H17A—C17—H17B	109.5
C11—C10—C8	115.3 (3)	C16—C17—H17C	109.5
C11—C10—H10A	108.5	H17A—C17—H17C	109.5
C8—C10—H10A	108.5	H17B—C17—H17C	109.5
C11—C10—H10B	108.5	C7—N1—C1	120.2 (2)
C8—C10—H10B	108.5	C7—N2—C8	112.1 (2)
H10A—C10—H10B	107.5	C7—N2—H2A	122.5
C10—C11—C12	112.9 (4)	C8—N2—H2A	116.7
C10—C11—C13	110.5 (4)	N2—C8—C10	113.9 (3)
C12—C11—C13	109.9 (4)	N2—C8—C9	102.5 (2)
C10—C11—H11	107.8	C10—C8—C9	109.7 (2)
C12—C11—H11	107.8	N2—C8—H8	110.2
C13—C11—H11	107.8	C10—C8—H8	110.2
C11—C12—H12A	109.5	C9—C8—H8	110.2
C11—C12—H12B	109.5	C9—N3—C7	112.8 (2)
H12A—C12—H12B	109.5	C9—N3—C14	124.3 (2)
C11—C12—H12C	109.5	C7—N3—C14	122.5 (2)
H12A—C12—H12C	109.5	C15—O3—C16	117.8 (3)
H12B—C12—H12C	109.5		

C6—C1—C2—C3	−0.7 (4)	C11—C10—C8—N2	−68.4 (4)
N1—C1—C2—C3	−175.0 (3)	C11—C10—C8—C9	177.5 (3)
C1—C2—C3—C4	0.7 (5)	O1—C9—C8—N2	177.5 (3)
C2—C3—C4—C5	0.1 (5)	N3—C9—C8—N2	−5.4 (3)
C3—C4—C5—C6	−1.0 (5)	O1—C9—C8—C10	−61.2 (4)
C2—C1—C6—C5	−0.2 (4)	N3—C9—C8—C10	115.9 (3)
N1—C1—C6—C5	174.0 (3)	O1—C9—N3—C7	−174.2 (3)
C4—C5—C6—C1	1.0 (5)	C8—C9—N3—C7	8.6 (3)
C8—C10—C11—C12	−62.8 (5)	O1—C9—N3—C14	−0.6 (5)
C8—C10—C11—C13	173.7 (4)	C8—C9—N3—C14	−177.7 (2)
N3—C14—C15—O2	12.5 (5)	N1—C7—N3—C9	173.8 (3)
N3—C14—C15—O3	−168.6 (3)	N2—C7—N3—C9	−8.3 (3)
N2—C7—N1—C1	8.7 (5)	N1—C7—N3—C14	0.1 (4)
N3—C7—N1—C1	−174.1 (2)	N2—C7—N3—C14	177.9 (2)
C6—C1—N1—C7	63.9 (4)	C15—C14—N3—C9	−94.3 (3)
C2—C1—N1—C7	−122.0 (3)	C15—C14—N3—C7	78.7 (3)
N1—C7—N2—C8	−178.2 (3)	O2—C15—O3—C16	1.9 (5)
N3—C7—N2—C8	4.3 (3)	C14—C15—O3—C16	−177.1 (3)
C7—N2—C8—C10	−117.7 (3)	C17—C16—O3—C15	85.4 (5)
C7—N2—C8—C9	0.6 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2^{i}	0.93	2.47	3.257 (4)	143
N2—H2A···O1^{i}	0.86	2.31	3.137 (3)	162

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

Fig. 1

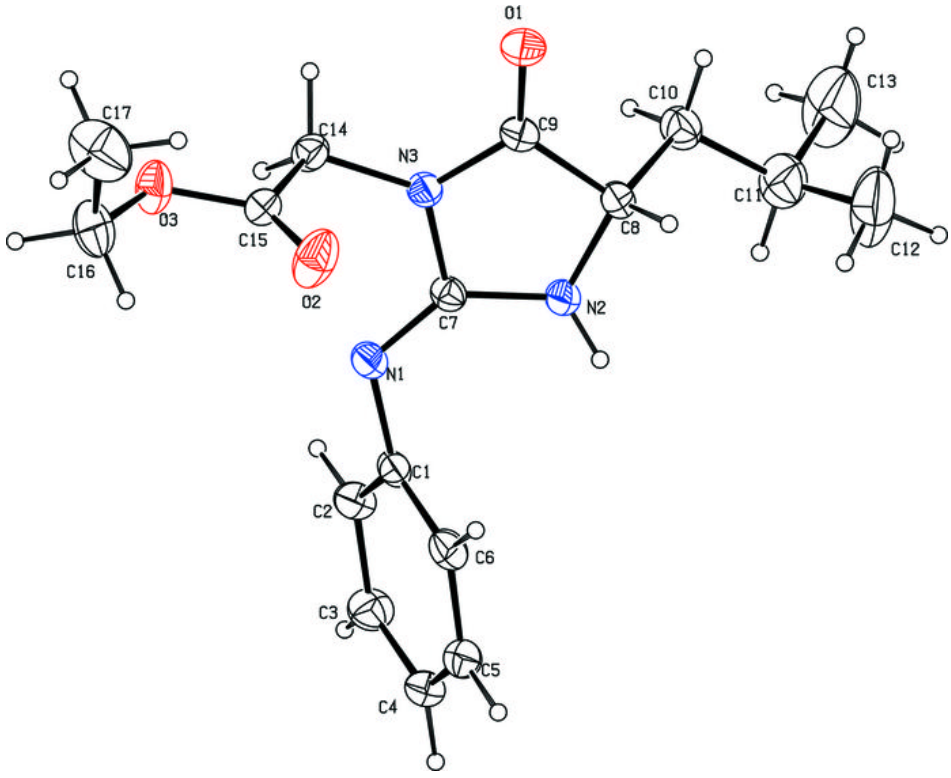
O1
C17
C14
N3
C9
C10
C13
O3
C15
C8
C11
C16
O2
C7
N2
C12
N1
C1
C2
C6
C3
C5
C4

Fig. 2

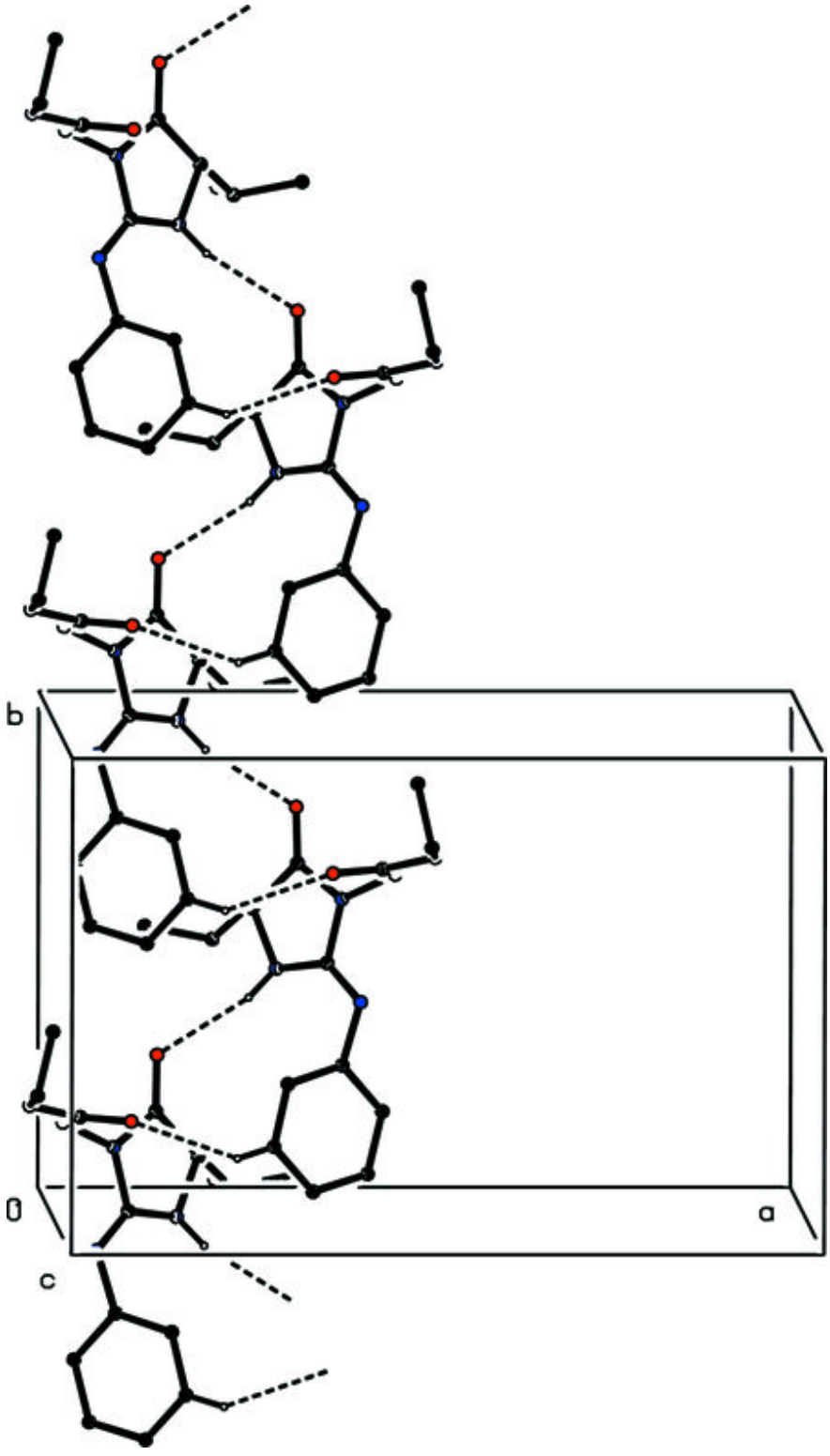

Fig. 3