Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-[3-(3-Fluorophenyl)-1,2,4-oxadiazol-5-yl]propionic acid

Suseanne K. M. Santos,[a] Ricardo A. W. Neves Filho,[a] Adailton J. Bortoluzzi[b] and Rajendra M. Srivastava[a]*

[a]Depto. de Química Fundamental, Universidade Federal de Pernambuco, 50740-540 Recife, Pernambuco, Brazil, and [b]Depto. de Química, Universidade Federal de Santa Catarina, 88040-900 Florianópolis, Santa Catarina, Brazil
Correspondence e-mail: rms_indu@yahoo.com

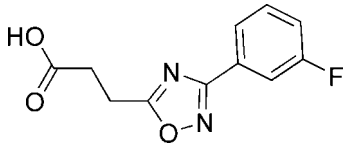
Received 18 November 2008; accepted 10 December 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.112; data-to-parameter ratio = 13.1.

In the title compound, $C_{11}H_9FN_2O_3$, the benzene ring is almost coplanar with the heterocyclic ring, making a dihedral angle of 14.0 (1)°. The plane of the carboxyl group is rotated by 14.7 (3)° with respect to the 1,2,4-oxadiazole ring plane. The aliphatic chain exhibits a standard zigzag arrangement. Two intermolecular O—H···O hydrogen bonds between the carboxyl groups related by an inversion centre promote a dimeric structure formation. The dimers are stacked along the crystallographic *a* axis.

Related literature

For general background, see: Gallardo *et al.* (2008); Jakopin & Dolenc (2008). For related structures, see: Wang *et al.* (2006, 2007); Yan, Xing *et al.* (2006); Yan *et al.* (2006*a*,*b*). For the method of preparation, see: Sindkhedkar *et al.* (2008); Srivastava & Seabra (1997).



Experimental

Crystal data

$C_{11}H_9FN_2O_3$
M_r = 236.20
Triclinic, $P\overline{1}$
a = 5.055 (1) Å
b = 5.905 (1) Å
c = 17.967 (1) Å
α = 85.769 (5)°
β = 87.965 (7)°
γ = 81.252 (7)°
V = 528.47 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 293 (2) K
0.50 × 0.33 × 0.07 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
2136 measured reflections
2066 independent reflections
1557 reflections with $I > 2\sigma(I)$
R_{int} = 0.010
3 standard reflections
every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.112
S = 1.06
2066 reflections
158 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 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
O10—H10···O9^{i}	0.97 (3)	1.68 (3)	2.650 (2)	179 (3)

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *HELENA* (Spek, 1996); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

The authors are grateful to the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) for financial assistance. SKMS thanks the Programa Institucional de Bolsas de Iniciação Científica (PIBIC/CNPq) for an Undergraduate fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2367).

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Enraf–Nonius (1989). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
Gallardo, H., Cristiano, R., Vieira, A. A., Neves Filho, R. A. W. & Srivastava, R. M. (2008). *Synthesis*, pp. 605–609.
Jakopin, Z. & Dolenc, M. S. (2008). *Curr. Org. Chem.* **12**, 850–898.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sindkhedkar, M. D., Desai, V. N., Loriya, R. M., Patel, M. V., Trivedi, B. K., Bora, R. O., Diwakar, S. D., Jadhav, G. R. & Pawar, S. S. (2008). PCT Int. Patent Appl. 123pp.
Spek, A. L. (1996). *HELENA*. University of Utrecht, The Netherlands.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Srivastava, R. M. & Seabra, G. M. (1997). *J. Braz. Chem. Soc.* **8**, 397–405.
Wang, P., Li, H., Kang, S. & Wang, H. (2007). *Acta Cryst.* E**63**, o4411.
Wang, H.-B., Liu, Z.-Q., Wang, H.-B. & Yan, X.-C. (2006). *Acta Cryst.* E**62**, o4715–o4716.
Yan, X.-C., Wang, H.-B. & Liu, Z.-Q. (2006*a*). *Acta Cryst.* E**62**, o3007–o3008.
Yan, X.-C., Wang, H.-B. & Liu, Z.-Q. (2006*b*). *Acta Cryst.* E**62**, o1302–o1303.
Yan, X.-C., Xing, Z.-T., Liu, Z.-Q. & Wang, H.-B. (2006). *Acta Cryst.* E**62**, o4640–o4641.

supporting information

Acta Cryst. (2009). E**65**, o146 [doi:10.1107/S1600536808042001]

3-[3-(3-Fluorophenyl)-1,2,4-oxadiazol-5-yl]propionic acid

Suseanne K. M. Santos, Ricardo A. W. Neves Filho, Adailton J. Bortoluzzi and Rajendra M. Srivastava

S1. Comment

1,2,4-Oxadiazoles are well known compounds, which exhibit a large number of biological activities (Jakopin & Dolenc, 2008). Recently, the use of this heterocycle as core for luminescent liquid crystals has also been described (Gallardo *et al.*, 2008).

In the title compound (Fig. 1), the bond lengths and angles are in agreement with the values previously reported for 1,2,4-oxadiazole-containing molecules (Wang *et al.*, 2006, 2007; Yan, Xing *et al.*, 2006; Yan *et al.*, 2006*a*,*b*). The torsion angle N2—C3—C11—C16 between the benzene ring attached to C-3 of the 1,2,4-oxadiazole system is -13.6 (2)°, thus, both rings are almost coplanar. The C-5 side-chain containing a carboxylic acid group shows a zigzag arrangement, having the torsion angle C5—C6—C7—C8 of -179.4 (1)°. In addition, the plane of the carboxylic group is also rotated by 14.7 (3)° with respect to the mean plane of the 1,2,4-oxadiazole five-membered ring, but in opposite direction of deviation of the fluoro-phenyl ring. This makes the molecular structure to be slightly twisted. Carboxylic groups are involved in centrosymmetric intermolecular hydrogen-bonding forming a dimeric structure (Fig. 2). The dimmers are perfectly stacked along the crystallographic *a* axis (Fig. 3).

S2. Experimental

The title compound was synthesized following the procedure reported earlier for the analogous compounds (Srivastava & Seabra, 1997; Sindkhedkar *et al.*, 2008). A mixture of 3-fluorbenzamidoxime (2.0 mmol) and succinic anhydride (2.2 mmol) was heated in a domestic microwave oven for 10 min. The crude material was purified by column chromatography. Crystallization of pure material from chloroform, from which a suitable crystal was chosen for the X-ray crystallographic experiment.

S3. Refinement

H atoms attached to C atoms were added at their calculated positions and included in the structure factors calculations, with C—H = 0.93 (aromatic) and 0.97 Å (methylene), and with U_{iso}(H) = 1.2U_{eq}(C). The H atom of carboxylic acid was located in a difference Fourier map and treated as a free atom.

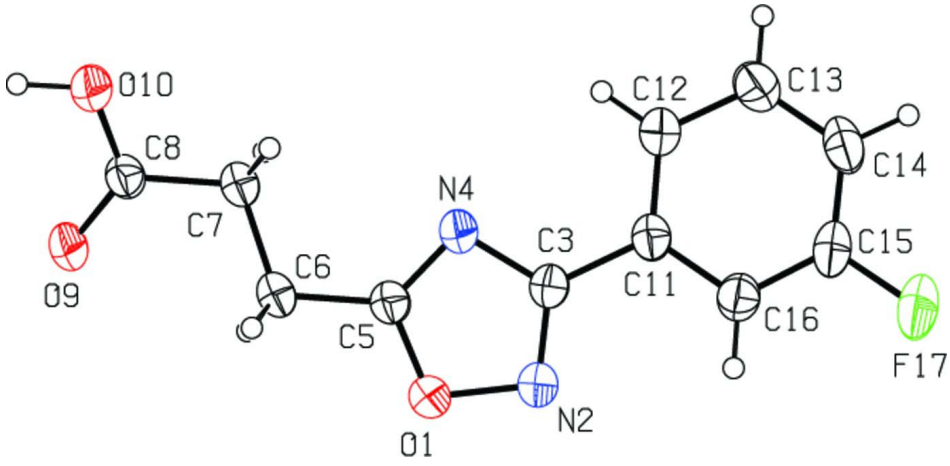


Figure 1

The molecular structure of (I) with labeling scheme. Displacement ellipsoids are shown at the 40% probability level.

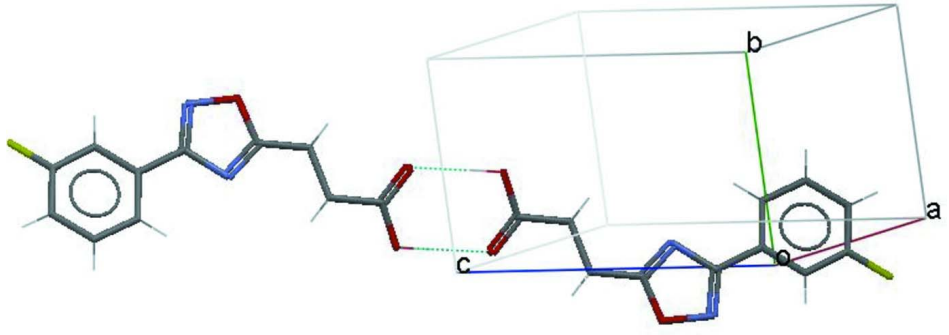


Figure 2

Dimeric strucuture formed by hydrogen bonding.

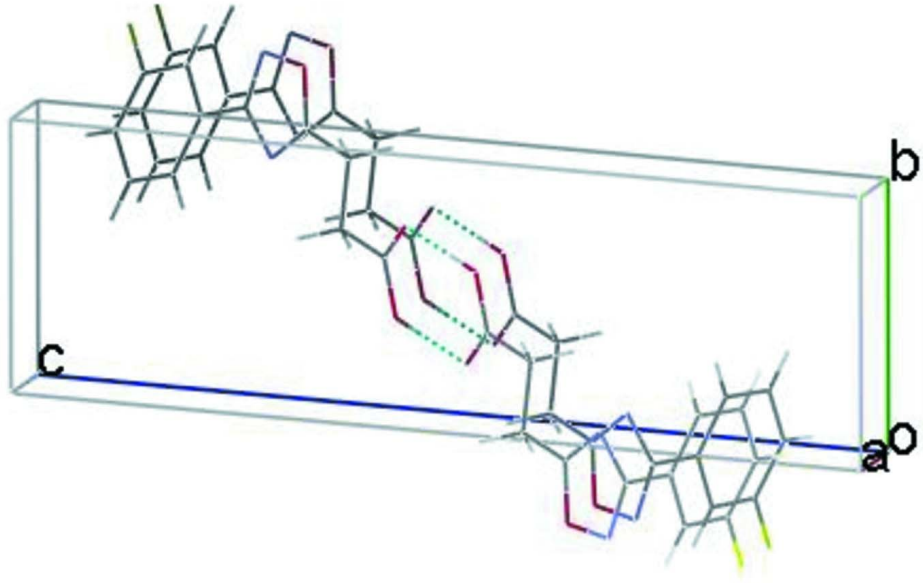


Figure 3

Molecules of (I) stacked along the *a* axis.

3-[3-(3-Fluorophenyl)-1,2,4-oxadiazol-5-yl]propionic acid

Crystal data

$C_{11}H_9FN_2O_3$
$M_r = 236.20$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.055$ (1) Å
$b = 5.905$ (1) Å
$c = 17.967$ (1) Å
$\alpha = 85.769$ (5)°
$\beta = 87.965$ (7)°
$\gamma = 81.252$ (7)°
$V = 528.47$ (14) Å^3
$Z = 2$
$F(000) = 244$
$D_x = 1.484$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 5.0$–18.8°
$\mu = 0.12$ mm^{-1}
$T = 293$ K
Irregular plate, colorless
0.50 × 0.33 × 0.07 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω–2θ scans
2136 measured reflections
2066 independent reflections
1557 reflections with $I > 2\sigma(I)$
$R_{int} = 0.010$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.1°$
$h = -6 \rightarrow 6$
$k = -7 \rightarrow 7$
$l = -22 \rightarrow 0$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.112$
$S = 1.06$
2066 reflections
158 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.0868P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H atoms treated by a mixture of independent and constrained refinement	$\Delta\rho_{max} = 0.21$ e Å^{-3}
	$\Delta\rho_{min} = -0.21$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C3	0.1073 (3)	−0.0359 (3)	0.24108 (9)	0.0403 (4)
C5	−0.1973 (3)	0.0022 (3)	0.32245 (9)	0.0412 (4)
C6	−0.4105 (3)	0.0731 (3)	0.37879 (10)	0.0463 (4)
H6A	−0.3429	0.0278	0.4284	0.056*
H6B	−0.5616	−0.0064	0.3722	0.056*
C7	−0.5043 (3)	0.3291 (3)	0.37270 (10)	0.0476 (4)
H7A	−0.3529	0.4086	0.3788	0.057*
H7B	−0.5738	0.3741	0.3233	0.057*
C8	−0.7169 (3)	0.4009 (3)	0.42998 (9)	0.0422 (4)
C11	0.3022 (3)	0.0236 (3)	0.18257 (9)	0.0415 (4)
C12	0.2778 (4)	0.2461 (3)	0.15009 (10)	0.0522 (4)
H12	0.1426	0.3584	0.1660	0.063*
C13	0.4575 (4)	0.2996 (4)	0.09349 (11)	0.0618 (5)
H13	0.4413	0.4485	0.0715	0.074*
C14	0.6588 (4)	0.1352 (4)	0.06958 (11)	0.0594 (5)
H14	0.7785	0.1708	0.0316	0.071*
C15	0.6783 (3)	−0.0823 (3)	0.10322 (10)	0.0534 (5)
C16	0.5063 (3)	−0.1432 (3)	0.15924 (10)	0.0483 (4)
H16	0.5256	−0.2923	0.1811	0.058*
N2	0.0849 (3)	−0.2473 (3)	0.26222 (9)	0.0552 (4)
N4	−0.0667 (3)	0.1270 (2)	0.27700 (8)	0.0437 (3)
O1	−0.1230 (2)	−0.2237 (2)	0.31750 (7)	0.0555 (4)
O9	−0.8599 (2)	0.2685 (2)	0.45969 (7)	0.0547 (3)
O10	−0.7395 (3)	0.6168 (2)	0.44456 (8)	0.0551 (3)
F17	0.8776 (2)	−0.2448 (2)	0.07982 (7)	0.0822 (4)
H10	−0.885 (6)	0.660 (5)	0.4800 (16)	0.102 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C3	0.0353 (8)	0.0424 (8)	0.0424 (8)	−0.0037 (6)	0.0030 (7)	−0.0040 (7)
C5	0.0372 (8)	0.0418 (8)	0.0440 (9)	−0.0059 (6)	0.0037 (7)	−0.0008 (7)
C6	0.0424 (9)	0.0479 (9)	0.0476 (9)	−0.0091 (7)	0.0116 (7)	0.0011 (7)
C7	0.0432 (9)	0.0465 (9)	0.0510 (10)	−0.0062 (7)	0.0137 (7)	0.0019 (7)
C8	0.0359 (8)	0.0454 (9)	0.0442 (9)	−0.0060 (7)	0.0050 (7)	0.0014 (7)
C11	0.0373 (8)	0.0482 (9)	0.0402 (8)	−0.0093 (7)	0.0040 (6)	−0.0076 (7)
C12	0.0533 (10)	0.0504 (10)	0.0511 (10)	−0.0047 (8)	0.0130 (8)	−0.0059 (8)
C13	0.0734 (13)	0.0582 (12)	0.0543 (11)	−0.0167 (10)	0.0160 (9)	−0.0023 (9)
C14	0.0573 (11)	0.0746 (14)	0.0489 (10)	−0.0210 (10)	0.0186 (9)	−0.0092 (9)

C15	0.0414 (9)	0.0669 (12)	0.0518 (10)	−0.0044 (8)	0.0114 (8)	−0.0165 (9)
C16	0.0445 (9)	0.0497 (10)	0.0503 (10)	−0.0057 (7)	0.0045 (8)	−0.0070 (7)
N2	0.0529 (9)	0.0452 (8)	0.0633 (10)	−0.0008 (6)	0.0206 (7)	0.0004 (7)
N4	0.0412 (7)	0.0429 (7)	0.0468 (8)	−0.0076 (6)	0.0108 (6)	−0.0045 (6)
O1	0.0560 (7)	0.0418 (7)	0.0646 (8)	−0.0033 (5)	0.0208 (6)	0.0038 (5)
O9	0.0488 (7)	0.0519 (7)	0.0636 (8)	−0.0129 (5)	0.0229 (6)	−0.0052 (6)
O10	0.0517 (7)	0.0471 (7)	0.0665 (8)	−0.0103 (5)	0.0198 (6)	−0.0077 (6)
F17	0.0635 (7)	0.0919 (10)	0.0841 (9)	0.0081 (6)	0.0308 (6)	−0.0145 (7)

Geometric parameters (Å, º)

C3—N2	1.298 (2)	C11—C12	1.387 (2)
C3—N4	1.382 (2)	C11—C16	1.389 (2)
C3—C11	1.475 (2)	C12—C13	1.390 (3)
C5—N4	1.291 (2)	C12—H12	0.9300
C5—O1	1.338 (2)	C13—C14	1.376 (3)
C5—C6	1.486 (2)	C13—H13	0.9300
C6—C7	1.511 (2)	C14—C15	1.370 (3)
C6—H6A	0.9700	C14—H14	0.9300
C6—H6B	0.9700	C15—F17	1.359 (2)
C7—C8	1.497 (2)	C15—C16	1.370 (2)
C7—H7A	0.9700	C16—H16	0.9300
C7—H7B	0.9700	N2—O1	1.4183 (19)
C8—O9	1.2252 (19)	O10—H10	0.97 (3)
C8—O10	1.308 (2)		
N2—C3—N4	114.80 (14)	C12—C11—C3	119.61 (15)
N2—C3—C11	122.14 (14)	C16—C11—C3	120.18 (15)
N4—C3—C11	123.06 (14)	C11—C12—C13	119.36 (17)
N4—C5—O1	113.59 (14)	C11—C12—H12	120.3
N4—C5—C6	129.61 (15)	C13—C12—H12	120.3
O1—C5—C6	116.79 (13)	C14—C13—C12	120.87 (18)
C5—C6—C7	112.30 (13)	C14—C13—H13	119.6
C5—C6—H6A	109.1	C12—C13—H13	119.6
C7—C6—H6A	109.1	C15—C14—C13	118.25 (17)
C5—C6—H6B	109.1	C15—C14—H14	120.9
C7—C6—H6B	109.1	C13—C14—H14	120.9
H6A—C6—H6B	107.9	F17—C15—C14	118.33 (16)
C8—C7—C6	112.31 (14)	F17—C15—C16	118.68 (18)
C8—C7—H7A	109.1	C14—C15—C16	122.99 (17)
C6—C7—H7A	109.1	C15—C16—C11	118.33 (17)
C8—C7—H7B	109.1	C15—C16—H16	120.8
C6—C7—H7B	109.1	C11—C16—H16	120.8
H7A—C7—H7B	107.9	C3—N2—O1	102.97 (13)
O9—C8—O10	123.07 (15)	C5—N4—C3	102.40 (13)
O9—C8—C7	122.54 (15)	C5—O1—N2	106.23 (12)
O10—C8—C7	114.38 (14)	C8—O10—H10	112.6 (16)
C12—C11—C16	120.20 (15)		

N4—C5—C6—C7	8.6 (3)	C13—C14—C15—C16	0.2 (3)
O1—C5—C6—C7	−172.42 (15)	F17—C15—C16—C11	−179.68 (16)
C5—C6—C7—C8	−179.36 (14)	C14—C15—C16—C11	0.3 (3)
C6—C7—C8—O9	−23.4 (2)	C12—C11—C16—C15	−0.8 (3)
C6—C7—C8—O10	157.66 (15)	C3—C11—C16—C15	178.08 (15)
N2—C3—C11—C12	165.28 (17)	N4—C3—N2—O1	−0.10 (19)
N4—C3—C11—C12	−14.0 (2)	C11—C3—N2—O1	−179.48 (14)
N2—C3—C11—C16	−13.6 (2)	O1—C5—N4—C3	−0.79 (18)
N4—C3—C11—C16	167.08 (15)	C6—C5—N4—C3	178.25 (16)
C16—C11—C12—C13	0.7 (3)	N2—C3—N4—C5	0.54 (19)
C3—C11—C12—C13	−178.15 (17)	C11—C3—N4—C5	179.91 (15)
C11—C12—C13—C14	−0.2 (3)	N4—C5—O1—N2	0.77 (19)
C12—C13—C14—C15	−0.3 (3)	C6—C5—O1—N2	−178.40 (14)
C13—C14—C15—F17	−179.80 (17)	C3—N2—O1—C5	−0.37 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O10—H10···O9^{i}	0.97 (3)	1.68 (3)	2.650 (2)	179 (3)

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