Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Diethyl 2-[(3,5-dimethyl-1*H*-pyrazol-1-yl)(4-methoxyphenyl)methyl]propanedioate

Ihssan Meskini,[a] Maria Daoudi,[a]* Jean-Claude Daran,[b] Abdelali Kerbal[a] and Hafid Zouihri[c]

[a]Laboratoire de Chimie Organique, Faculté des Sciences Dhar el Mahraz, Université Sidi Mohammed Ben Abdellah, Fès, Morocco, [b]Laboratoire de Chimie de Coordination, 205 Route de Narbonne, 31077 Toulouse Cedex, France, and [c]Laboratoires de Diffraction des Rayons X, Division UATRS, Centre National pour la Recherche Scientifique et Technique, Rabat, Morocco
Correspondence e-mail: daoudimaria@yahoo.fr

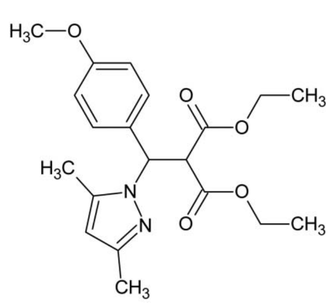
Received 26 June 2010; accepted 29 June 2010

Key indicators: single-crystal X-ray study; T = 296 K; P = 0.0 kPa; mean σ(C–C) = 0.003 Å; R factor = 0.056; wR factor = 0.154; data-to-parameter ratio = 15.7.

The title compound, $C_{20}H_{26}N_2O_5$, was prepared in good yield (76%) through condensation of diethyl (4-methoxybenzyl)propanedioate with 3,5-dimethyl-1*H*-pyrazole. The dihedral between the benzene and pyrazole rings is 83.96 (10)°. The crystal packing is stabilized by a C—H···O interaction, which links the molecules into centrosymmetric dimers.

Related literature

For related compounds displaying biological activity, see: Dayam *et al.* (2007); Patil *et al.* (2007); Ramkumar *et al.* (2008); Sechi *et al.* (2009) & Zeng *et al.* (2008). For the synthetic procedure, see: Pommier & Neamati (2006).



Experimental

Crystal data

$C_{20}H_{26}N_2O_5$
M_r = 374.43
Monoclinic, $P2_1/c$
a = 11.9618 (3) Å
b = 7.9681 (2) Å
c = 21.1269 (6) Å
β = 96.504 (1)°
V = 2000.70 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.23 × 0.17 × 0.14 mm

Data collection

Bruker X8 APEXII CCD area-detector diffractometer
18616 measured reflections
3921 independent reflections
3177 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.154
S = 1.05
3921 reflections
249 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O2^{i}	0.93	2.51	3.358 (3)	152

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

This work was supported by grants from Project PGR-UMP-BH-2005, the Centre National de Recherche Scientifique, CNRS (France), the Centre National pour la Recherche Scientifique et Technique, CNRST (Morocco), and the CURI (Morocco).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5280).

References

Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dayam, R., Al-Mawsawi, L. Q. & Neamati, N. (2007). *Bioorg. Med. Chem. Lett.* **17**, 6155–6159.
Patil, S., Kamath, S., Sanchez, T., Neamati, N., Schinazi, R. F. & Buolamwini, J. K. (2007). *Bioorg. Med. Chem.* **15**, 1212–1228.
Pommier, Y. & Neamati, N. (2006). *Bioorg. Med. Chem.* **14**, 3785–3792.
Ramkumar, K., Tambov, K. V., Gundla, R., Manaev, A. V., Yarovenko, V., Traven, V. F. & Neamati, N. (2008). *Bioorg. Med. Chem.* **16**, 8988–8998.
Sechi, M., Carta, F., Sannia, L., Dallocchio, R., Dessì, A., Al-Safi, R. I. & Neamati, N. (2009). *Antiviral Res.* **81**, 267–276.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**. Submitted.
Zeng, L. F., Zhang, H.-S. W., ang, Y. H., Sanchez, T., Zheng, Y. T., Neamati, N. & Long, Y. Q. (2008). *Bioorg. Med. Chem. Lett.* **18**, 4521–4524.

supplementary materials

Acta Cryst. (2010). E**66**, o1965 [doi:10.1107/S1600536810025572]

Diethyl 2-[(3,5-dimethyl-1*H*-pyrazol-1-yl)(4-methoxyphenyl)methyl]propanedioate

I. Meskini, M. Daoudi, J.-C. Daran, A. Kerbal and H. Zouihri

Comment

For the rational design of new HIV-1 Integrase (H—I) inhibitors, one validated target for chemotherapeutic intervention (Dayam *et al.,* 2007), is fundamentally based on intermolecular coordination between H—I / chemical inhibitor / metals (Mg^{+2} and Mn^{+2}, co-factors of the enzyme), leading to the formation of bimetallic complexes (Zeng *et al.,* 2008; Sechi *et al.*, 2009). Thereby, several bimetallic metal complexes, in many cases exploring the known-well polydentate ligands, appear in this scenario as the most promising concept to be employed in either enzyme / drug interaction or electron transfer process, in the last case involving the biological oxygen transfer (Sechi *et al.,* 2009; Ramkumar *et al.,* 2008). Another exciting example of application for such polydentate ligands involves the synergic water activation, that occurs *via* the so-called -remote metallic atoms. Such organometallic compounds are structurally deemed to promote or block the H—I activity (Zeng *et al.,* 2008).

In the molecule of the title compound (Fig.1), the dihedral angle between the planes of the pheny and the pyrazol ring is 83.96 (10)°.

Experimental

To a solution of the diethyl (4-methoxybenzyl)propanedioate (5 mmol) in water (20 ml) was added the 3,5-dimethyl-1*H*-pyrazole (6 mmol) and the mixture and the stirring was continued at room temperature until the complete consume of the starting material. After removing solvent, the crude products were dissolved in diethyl ether (2x40 ml) and washed with water until the pH became neutral. The organic solvent was dried with sodium sulfate and then evaporated to give the pure compound (I) with 76% yield.. White crystals are obtained by recrystallization in ether/hexane (2/1).

Suitable single-crystal of malonate derivative (I) was obtained by recrystallization from ethanol. A white-transparent crystal was mounted on a glass fibre.

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.96 Å (methyl), C—H = 0.93 Å (aromatic), 0.97 Å (methylene) and 0.98 Å (methine) with $U_{iso}(H) = 1.2U_{eq}$ or $U_{iso}(H) = 1.5U_{eq}$(methyl).

Figures

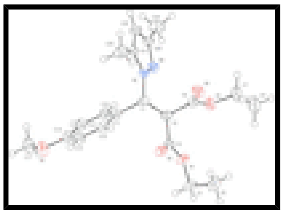


Fig. 1. Molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

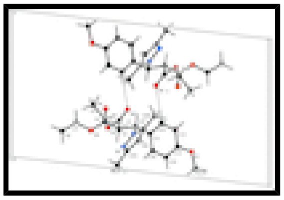


Fig. 2. Partial packing view showing the chain generated by C—H···O hydrogen bonds shown as dashed lines. Symmetry code for generating the second molecule: 1 - *x*,-*y*,1 - *z*.

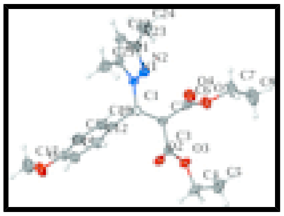


Fig. 3. View of the title compound showing displacement ellipsoids at the 50% probability level.

Diethyl 2-[(3,5-dimethyl-1*H*-pyrazol-1-yl)(4-methoxyphenyl)methyl]propanedioate

Crystal data

$C_{20}H_{26}N_2O_5$	$F(000) = 800$
$M_r = 374.43$	$D_x = 1.243$ Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 361 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 11.9618$ (3) Å	Cell parameters from 2174 reflections
$b = 7.9681$ (2) Å	$\theta = 2.3–27.1°$
$c = 21.1269$ (6) Å	$\mu = 0.09$ mm^{-1}
$\beta = 96.504$ (1)°	$T = 296$ K
$V = 2000.70$ (9) Å^3	Block, colourless
$Z = 4$	0.23 × 0.17 × 0.14 mm

Data collection

Bruker X8 APEXII CCD area-detector diffractometer	3177 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.027$
graphite	$\theta_{max} = 26.0°$, $\theta_{min} = 2.7°$
φ and ω scans	$h = -14 \rightarrow 14$
18616 measured reflections	$k = -9 \rightarrow 9$
3921 independent reflections	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.056$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.154$	H-atom parameters constrained
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0687P)^2 + 1.8319P]$ where $P = (F_o^2 + 2F_c^2)/3$
3921 reflections	$(\Delta/\sigma)_{max} = 0.007$
249 parameters	$\Delta\rho_{max} = 0.68$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.45$ e Å^{-3}

Special details

Experimental. The data collection nominally covered a sphere of reciprocal space, by a combination of tree sets of exposures; each set had a different φ angle for the crystal and each exposure covered 0.5° in ω and 20 s in time. The crystal-to-detector distance was 37.5 mm.

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 $F^2 > \sigma(F^2)$ 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}
O2	0.40914 (11)	−0.14261 (19)	0.44322 (7)	0.0301 (3)
O3	0.26937 (12)	−0.19794 (18)	0.36564 (7)	0.0321 (4)
O4	0.39768 (14)	0.2442 (2)	0.36381 (8)	0.0441 (4)
O5	0.23951 (15)	0.1580 (2)	0.30637 (7)	0.0446 (4)
O1	0.16987 (15)	−0.2065 (2)	0.68944 (8)	0.0468 (5)
N1	0.25069 (14)	0.3219 (2)	0.47437 (8)	0.0252 (4)
N2	0.15274 (14)	0.3525 (2)	0.43620 (8)	0.0297 (4)
C1	0.29918 (16)	0.1528 (2)	0.47752 (9)	0.0230 (4)
H1	0.3813	0.1633	0.4845	0.028*
C2	0.26772 (16)	0.0673 (3)	0.41296 (9)	0.0244 (4)
H2	0.1859	0.0541	0.4051	0.029*
C11	0.26097 (16)	0.0542 (2)	0.53261 (9)	0.0229 (4)
C3	0.32439 (16)	−0.1032 (2)	0.41081 (9)	0.0239 (4)
C12	0.33950 (17)	−0.0251 (3)	0.57616 (9)	0.0277 (4)
H12	0.4154	−0.0197	0.5706	0.033*

C21	0.28468 (17)	0.4563 (3)	0.51094 (10)	0.0285 (5)
C16	0.14790 (16)	0.0419 (3)	0.54174 (10)	0.0277 (4)
H16	0.0941	0.0929	0.5127	0.033*
C13	0.30680 (18)	−0.1116 (3)	0.62736 (10)	0.0323 (5)
H13	0.3605	−0.1643	0.6559	0.039*
C14	0.19347 (18)	−0.1206 (3)	0.63658 (10)	0.0311 (5)
C15	0.11364 (17)	−0.0445 (3)	0.59307 (10)	0.0312 (5)
H15	0.0376	−0.0515	0.5983	0.037*
C6	0.30985 (19)	0.1697 (3)	0.35912 (10)	0.0308 (5)
C23	0.12710 (18)	0.5105 (3)	0.44907 (11)	0.0322 (5)
C4	0.32363 (19)	−0.3556 (3)	0.35159 (12)	0.0370 (5)
H4A	0.2679	−0.4329	0.3314	0.044*
H4B	0.3575	−0.4063	0.3909	0.044*
C22	0.20634 (18)	0.5797 (3)	0.49546 (10)	0.0330 (5)
H22	0.2060	0.6874	0.5124	0.040*
C5	0.4121 (2)	−0.3243 (4)	0.30837 (11)	0.0466 (6)
H5A	0.3789	−0.2693	0.2704	0.070*
H5B	0.4442	−0.4292	0.2973	0.070*
H5C	0.4699	−0.2542	0.3296	0.070*
C25	0.3888 (2)	0.4563 (3)	0.55689 (12)	0.0416 (6)
H25A	0.3743	0.4000	0.5953	0.062*
H25B	0.4114	0.5699	0.5666	0.062*
H25C	0.4478	0.3990	0.5384	0.062*
C7	0.2781 (3)	0.2351 (4)	0.24975 (12)	0.0612 (8)
H7A	0.2695	0.3560	0.2515	0.073*
H7B	0.3571	0.2098	0.2481	0.073*
C24	0.0258 (2)	0.5924 (3)	0.41410 (14)	0.0489 (7)
H24A	0.0493	0.6722	0.3842	0.073*
H24B	−0.0160	0.6490	0.4439	0.073*
H24C	−0.0209	0.5086	0.3917	0.073*
C17	0.0566 (2)	−0.2040 (4)	0.70479 (13)	0.0545 (7)
H17A	0.0335	−0.0900	0.7101	0.082*
H17B	0.0521	−0.2649	0.7436	0.082*
H17C	0.0081	−0.2554	0.6709	0.082*
C8	0.2127 (3)	0.1700 (5)	0.19471 (13)	0.0731 (10)
H8A	0.2245	0.0511	0.1922	0.110*
H8B	0.2351	0.2230	0.1573	0.110*
H8C	0.1345	0.1919	0.1975	0.110*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0249 (7)	0.0292 (8)	0.0357 (8)	0.0049 (6)	0.0007 (6)	−0.0048 (6)
O3	0.0317 (8)	0.0265 (8)	0.0371 (8)	0.0009 (6)	−0.0005 (6)	−0.0089 (6)
O4	0.0466 (10)	0.0436 (10)	0.0435 (9)	−0.0125 (8)	0.0117 (8)	0.0046 (8)
O5	0.0624 (11)	0.0441 (10)	0.0264 (8)	−0.0085 (8)	0.0010 (7)	0.0036 (7)
O1	0.0475 (10)	0.0586 (12)	0.0360 (9)	−0.0031 (9)	0.0117 (7)	0.0143 (8)
N1	0.0258 (8)	0.0229 (9)	0.0265 (8)	0.0027 (7)	0.0013 (7)	−0.0005 (7)

N2	0.0280 (9)	0.0278 (9)	0.0330 (9)	0.0061 (7)	0.0015 (7)	0.0008 (7)
C1	0.0216 (9)	0.0196 (9)	0.0277 (10)	0.0025 (7)	0.0022 (7)	−0.0011 (8)
C2	0.0221 (9)	0.0238 (10)	0.0273 (10)	0.0019 (8)	0.0031 (8)	−0.0012 (8)
C11	0.0242 (9)	0.0203 (10)	0.0246 (9)	0.0011 (8)	0.0036 (7)	−0.0037 (7)
C3	0.0230 (10)	0.0237 (10)	0.0257 (9)	−0.0028 (8)	0.0067 (8)	−0.0018 (8)
C12	0.0228 (10)	0.0311 (11)	0.0287 (10)	0.0005 (8)	0.0009 (8)	−0.0014 (8)
C21	0.0320 (11)	0.0253 (11)	0.0294 (10)	−0.0012 (8)	0.0088 (8)	−0.0025 (8)
C16	0.0242 (10)	0.0293 (11)	0.0292 (10)	0.0060 (8)	0.0014 (8)	−0.0008 (8)
C13	0.0315 (11)	0.0372 (13)	0.0268 (10)	0.0019 (9)	−0.0022 (8)	0.0033 (9)
C14	0.0379 (12)	0.0310 (12)	0.0253 (10)	−0.0017 (9)	0.0073 (9)	0.0011 (8)
C15	0.0255 (10)	0.0350 (12)	0.0340 (11)	0.0006 (9)	0.0078 (8)	−0.0019 (9)
C6	0.0405 (12)	0.0244 (11)	0.0277 (10)	0.0041 (9)	0.0041 (9)	−0.0028 (8)
C23	0.0340 (11)	0.0253 (11)	0.0385 (11)	0.0075 (9)	0.0100 (9)	0.0030 (9)
C4	0.0369 (12)	0.0279 (11)	0.0454 (13)	0.0010 (9)	0.0015 (10)	−0.0159 (10)
C22	0.0401 (12)	0.0222 (10)	0.0384 (12)	0.0037 (9)	0.0122 (10)	−0.0033 (9)
C5	0.0504 (15)	0.0548 (16)	0.0350 (12)	0.0052 (12)	0.0069 (11)	−0.0127 (12)
C25	0.0425 (13)	0.0381 (13)	0.0423 (13)	−0.0001 (11)	−0.0034 (10)	−0.0091 (11)
C7	0.097 (2)	0.0572 (18)	0.0293 (13)	−0.0235 (17)	0.0078 (14)	0.0054 (12)
C24	0.0432 (14)	0.0413 (15)	0.0613 (16)	0.0180 (11)	0.0019 (12)	0.0046 (13)
C17	0.0596 (17)	0.0595 (18)	0.0492 (15)	−0.0086 (14)	0.0274 (13)	0.0059 (13)
C8	0.113 (3)	0.072 (2)	0.0346 (14)	−0.033 (2)	0.0104 (16)	−0.0004 (14)

Geometric parameters (Å, °)

O2—C3	1.199 (2)	C13—H13	0.9300
O3—C3	1.331 (2)	C14—C15	1.388 (3)
O3—C4	1.460 (3)	C15—H15	0.9300
O4—C6	1.201 (3)	C23—C22	1.397 (3)
O5—C6	1.322 (3)	C23—C24	1.496 (3)
O5—C7	1.465 (3)	C4—C5	1.495 (3)
O1—C14	1.367 (3)	C4—H4A	0.9700
O1—C17	1.428 (3)	C4—H4B	0.9700
N1—C21	1.355 (3)	C22—H22	0.9300
N1—N2	1.367 (2)	C5—H5A	0.9600
N1—C1	1.466 (2)	C5—H5B	0.9600
N2—C23	1.331 (3)	C5—H5C	0.9600
C1—C11	1.517 (3)	C25—H25A	0.9600
C1—C2	1.533 (3)	C25—H25B	0.9600
C1—H1	0.9800	C25—H25C	0.9600
C2—C3	1.521 (3)	C7—C8	1.424 (4)
C2—C6	1.531 (3)	C7—H7A	0.9700
C2—H2	0.9800	C7—H7B	0.9700
C11—C12	1.390 (3)	C24—H24A	0.9600
C11—C16	1.391 (3)	C24—H24B	0.9600
C12—C13	1.376 (3)	C24—H24C	0.9600
C12—H12	0.9300	C17—H17A	0.9600
C21—C22	1.372 (3)	C17—H17B	0.9600
C21—C25	1.490 (3)	C17—H17C	0.9600
C16—C15	1.385 (3)	C8—H8A	0.9600

C16—H16	0.9300	C8—H8B	0.9600
C13—C14	1.393 (3)	C8—H8C	0.9600
C3—O3—C4	116.03 (16)	N2—C23—C24	120.3 (2)
C6—O5—C7	115.4 (2)	C22—C23—C24	128.4 (2)
C14—O1—C17	117.87 (19)	O3—C4—C5	110.0 (2)
C21—N1—N2	112.18 (17)	O3—C4—H4A	109.7
C21—N1—C1	127.50 (16)	C5—C4—H4A	109.7
N2—N1—C1	119.92 (16)	O3—C4—H4B	109.7
C23—N2—N1	104.46 (17)	C5—C4—H4B	109.7
N1—C1—C11	111.05 (15)	H4A—C4—H4B	108.2
N1—C1—C2	108.18 (15)	C21—C22—C23	105.97 (19)
C11—C1—C2	112.80 (16)	C21—C22—H22	127.0
N1—C1—H1	108.2	C23—C22—H22	127.0
C11—C1—H1	108.2	C4—C5—H5A	109.5
C2—C1—H1	108.2	C4—C5—H5B	109.5
C3—C2—C6	105.57 (15)	H5A—C5—H5B	109.5
C3—C2—C1	110.98 (16)	C4—C5—H5C	109.5
C6—C2—C1	110.86 (16)	H5A—C5—H5C	109.5
C3—C2—H2	109.8	H5B—C5—H5C	109.5
C6—C2—H2	109.8	C21—C25—H25A	109.5
C1—C2—H2	109.8	C21—C25—H25B	109.5
C12—C11—C16	118.10 (18)	H25A—C25—H25B	109.5
C12—C11—C1	120.23 (17)	C21—C25—H25C	109.5
C16—C11—C1	121.66 (17)	H25A—C25—H25C	109.5
O2—C3—O3	125.32 (19)	H25B—C25—H25C	109.5
O2—C3—C2	124.59 (18)	C8—C7—O5	108.6 (2)
O3—C3—C2	110.01 (16)	C8—C7—H7A	110.0
C13—C12—C11	121.13 (19)	O5—C7—H7A	110.0
C13—C12—H12	119.4	C8—C7—H7B	110.0
C11—C12—H12	119.4	O5—C7—H7B	110.0
N1—C21—C22	106.12 (18)	H7A—C7—H7B	108.3
N1—C21—C25	123.09 (19)	C23—C24—H24A	109.5
C22—C21—C25	130.8 (2)	C23—C24—H24B	109.5
C15—C16—C11	121.46 (19)	H24A—C24—H24B	109.5
C15—C16—H16	119.3	C23—C24—H24C	109.5
C11—C16—H16	119.3	H24A—C24—H24C	109.5
C12—C13—C14	120.21 (19)	H24B—C24—H24C	109.5
C12—C13—H13	119.9	O1—C17—H17A	109.5
C14—C13—H13	119.9	O1—C17—H17B	109.5
O1—C14—C15	124.7 (2)	H17A—C17—H17B	109.5
O1—C14—C13	115.74 (19)	O1—C17—H17C	109.5
C15—C14—C13	119.52 (19)	H17A—C17—H17C	109.5
C16—C15—C14	119.56 (19)	H17B—C17—H17C	109.5
C16—C15—H15	120.2	C7—C8—H8A	109.5
C14—C15—H15	120.2	C7—C8—H8B	109.5
O4—C6—O5	124.9 (2)	H8A—C8—H8B	109.5
O4—C6—C2	124.10 (19)	C7—C8—H8C	109.5
O5—C6—C2	110.92 (18)	H8A—C8—H8C	109.5
N2—C23—C22	111.27 (19)	H8B—C8—H8C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O2^{i}	0.93	2.51	3.358 (3)	152

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

Fig. 1

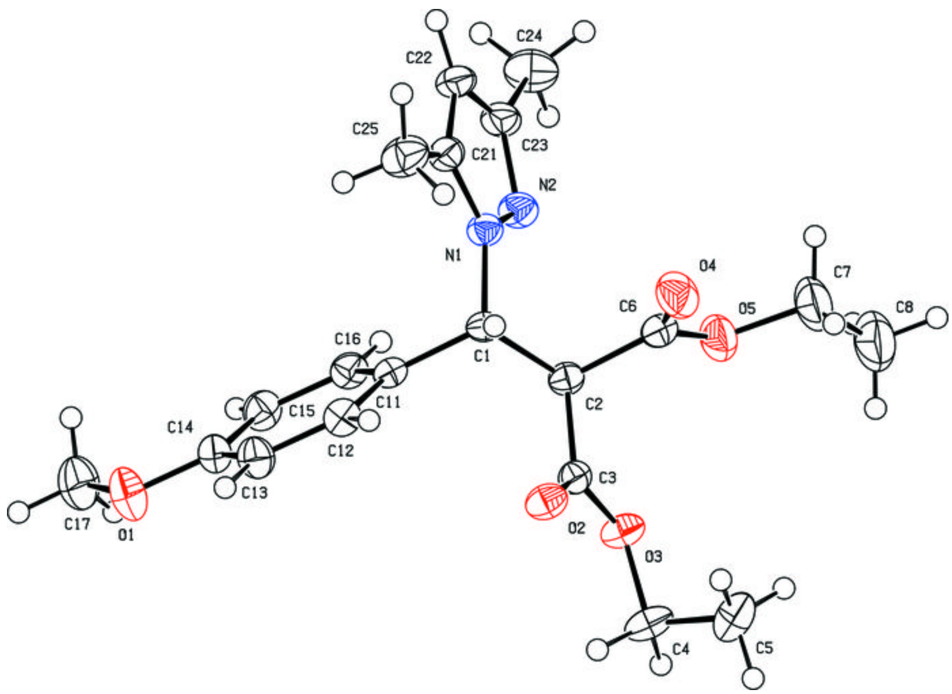

C24
C22
C25
C21
C23
N2
N1
O4
C7
C6
O5
C8
C16
C1
C11
C2
C15
C14
C12
C3
C13
C17
O1
O2
O3
C4
C5

Fig. 2

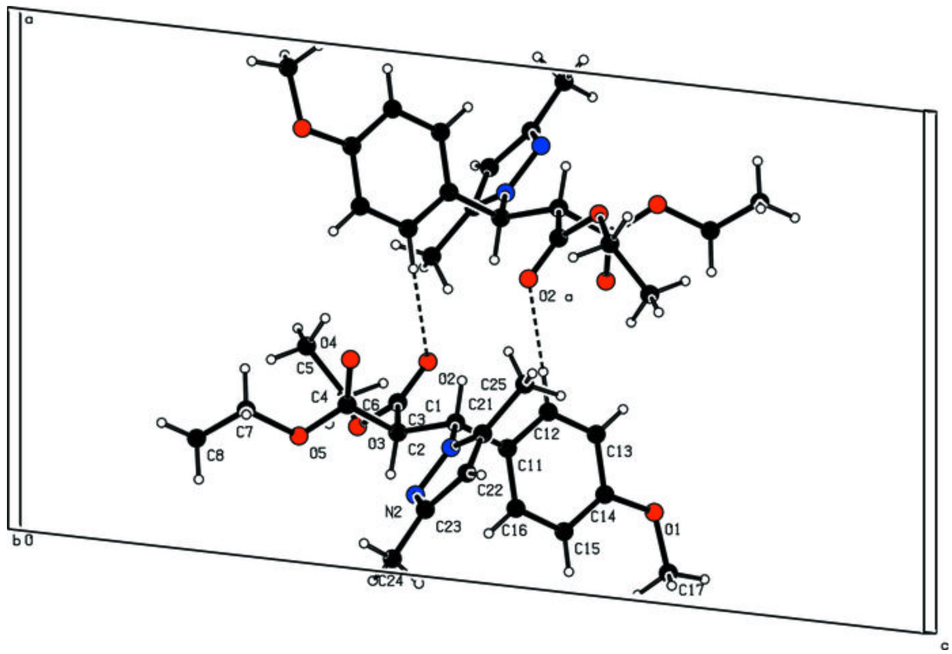

a
O2 a
O4
C5
C4
C6
O2
C1
C25
C21
C3
C7
C8
O5
O3
C2
C12
C13
C11
N2
C22
C23
C16
C14
O1
C15
C24
C17
b 0
c

Fig. 3