

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Editors: W. Clegg and D. G. Watson

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3,5-Di-*p*-toluoyl-1,2-dideoxy- β -1-(imidazol-1-yl)-D-ribofuranose

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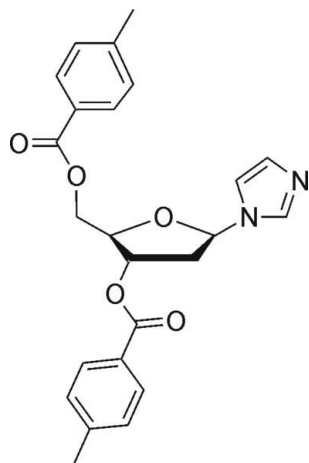
Received 2 November 2007; accepted 7 November 2007

Key indicators: single-crystal X-ray study; $T = 103$ K; mean $\sigma(\text{C}—\text{C}) = 0.006$ Å; R factor = 0.060; wR factor = 0.137; data-to-parameter ratio = 9.5.

The title compound, $\text{C}_{24}\text{H}_{24}\text{N}_2\text{O}_5$, was obtained as a reaction intermediate in the synthesis of the artificial imidazole nucleoside, which is a highly useful synthetic nucleoside for the formation of metal-ion-mediated base pairs. Compared to the free nucleoside, both OH groups of the sugar moiety are protected by *p*-toluoyl groups. The sugar is in its $\text{C3}'\text{-endo}$ conformation.

Related literature

The structures of the analogous 1,2,4-triazole and tetrazole nucleosides have been reported recently (Müller *et al.*, 2005). These nucleosides have been used in metal-ion-mediated base pairs (Böhme *et al.*, 2007). For related literature, see: Polonius & Müller (2007); Müller *et al.* (2007); Allen *et al.* (1987); Farrugia (1997, 1999).



Experimental

Crystal data

$\text{C}_{24}\text{H}_{24}\text{N}_2\text{O}_5$
 $M_r = 420.45$
Monoclinic, $P2_1$
 $a = 14.436$ (3) Å
 $b = 5.3850$ (11) Å
 $c = 15.061$ (3) Å
 $\beta = 116.25$ (3)°
 $V = 1050.1$ (5) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 103$ (2) K
0.1 × 0.1 × 0.1 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: none
12891 measured reflections
2647 independent reflections
1726 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.097$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$
 $wR(F^2) = 0.137$
 $S = 1.01$
2647 reflections
280 parameters
1 restraint
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.28$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.34$ e Å⁻³

Data collection: *KappaCCD* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Deutsche Forschungsgemeinschaft, the Department of Chemistry at the University of Dortmund and the Fonds der Chemischen Industrie.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2551).

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supplementary materials

Acta Cryst. (2007). E63, o4693 [doi:10.1107/S1600536807056760]

3,5-Di-*p*-toluoyl-1,2-dideoxy- β -1-(imidazol-1-yl)-D-ribofuranose

N. Düpre, W.-Z. Shen, P. J. Sanz Miguel and J. Müller

Comment

In the course of our studies regarding the use of artificial azole nucleosides (azole = imidazole, 1,2,4-triazole, tetrazole) in metal-ion mediated base pairs (Böhme *et al.*, 2007; Müller *et al.*, 2007; Polonius & Müller, 2007; Müller *et al.*, 2005) we have isolated the title compound (Figure 1) as a reaction intermediate in the synthesis of imidazole nucleoside. It crystallizes in the same space group and with very similar unit-cell dimensions as the related triazole nucleoside (Müller *et al.*, 2005). All bond lengths and angles are within the normal range (Allen *et al.*, 1987). The artificial nucleobase is connected to the sugar moiety *via* an N-glycosidic bond. It is oriented *anti* with respect to the sugar. The deoxyribose adopts a C3'-*endo* conformation (phase angle of pseudorotation = 7.7 (5)°). The title compound forms long columns along the crystallographic *b* axis (Fig. 2). However, there is no π stacking between neighboring toluoyl rings that are related by the symmetry operator ($x, y + 1, z$). Instead, neighboring rings that are related by the symmetry operator ($1 - x, y + 1/2, 3 - z$) are oriented at an angle of 62.7 (2)° with respect to each other.

Experimental

The title compound was prepared as reported previously (Müller *et al.*, 2005). Single crystals suitable for X-ray measurement were obtained by crystallization from dichloromethane and cyclohexane with triethylamine at room temperature. A satisfactory elemental analysis was obtained: Calcd. for C₂₄H₂₄N₂O₅: C 68.6, H 5.8, N 6.7; found: C 68.2, H 6.2, N 6.6.

Refinement

In the absence of significant anomalous dispersion effects, a total of 1277 Friedel pairs have been merged during the final refinement.

Hydrogen atoms were included in the refinement at calculated positions with C—H = 0.95–1.00 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C})$ for methyl groups.

Figures

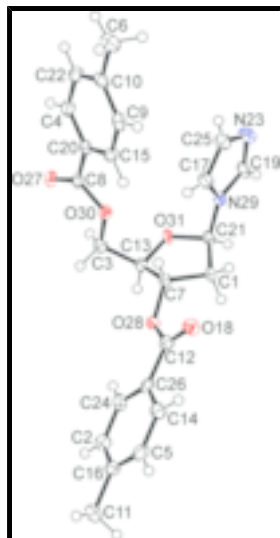


Fig. 1. View of the title compound showing displacement ellipsoids at the 50% probability level.

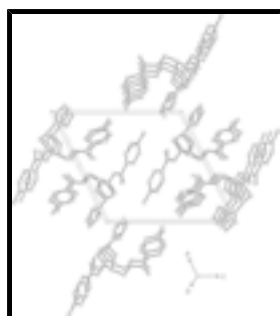


Fig. 2. Packing of the title compound with a view along the *b* axis.

3,5-Di-*p*-toluoxy-1,2-dideoxy- β -1-(imidazol-1-yl)-*D*-ribofuranose

Crystal data

$C_{24}H_{24}N_2O_5$

$M_r = 420.45$

Monoclinic, $P2_1$

Hall symbol: P 2yb

$a = 14.436 (3) \text{ \AA}$

$b = 5.3850 (11) \text{ \AA}$

$c = 15.061 (3) \text{ \AA}$

$\beta = 116.25 (3)^\circ$

$V = 1050.1 (5) \text{ \AA}^3$

$Z = 2$

$F_{000} = 444$

$D_x = 1.33 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

$\theta = 3\text{--}27.5^\circ$

$\mu = 0.09 \text{ mm}^{-1}$

$T = 103 (2) \text{ K}$

Cubes, colorless

$0.1 \times 0.1 \times 0.1 \text{ mm}$

Data collection

Bruker–Nonius Kappa CCD
diffractometer

profile fitted scans

$R_{\text{int}} = 0.097$

$\theta_{\text{max}} = 27.5^\circ$

Absorption correction: none	$\theta_{\min} = 3.0^\circ$
12891 measured reflections	$h = -18 \rightarrow 18$
2647 independent reflections	$k = -7 \rightarrow 5$
1726 reflections with $I > 2\sigma(I)$	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0694P)^2 + 0.2112P]$
	where $P = (F_o^2 + 2F_c^2)/3$
Least-squares matrix: full	$(\Delta/\sigma)_{\max} < 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.060$	$\Delta\rho_{\max} = 0.28 \text{ e } \text{\AA}^{-3}$
$wR(F^2) = 0.137$	$\Delta\rho_{\min} = -0.34 \text{ e } \text{\AA}^{-3}$
$S = 1.01$	Extinction correction: none
2647 reflections	
280 parameters	
1 restraint	
H-atom parameters constrained	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O30	0.3603 (2)	0.8395 (6)	0.96544 (19)	0.0222 (7)
N29	0.1239 (2)	1.0452 (6)	0.9936 (2)	0.0200 (8)
O28	0.44002 (19)	0.7940 (6)	1.24729 (19)	0.0221 (7)
O27	0.4201 (2)	0.9804 (6)	0.8587 (2)	0.0259 (7)
C26	0.5335 (3)	0.5234 (8)	1.3793 (3)	0.0200 (9)
C25	0.0239 (3)	0.8334 (9)	0.8628 (3)	0.0268 (10)
H25A	-0.0014	0.7064	0.8141	0.032*
C24	0.6206 (3)	0.6745 (9)	1.4091 (3)	0.0267 (11)
H24A	0.6179	0.822	1.3734	0.032*
N23	-0.0292 (3)	1.0479 (8)	0.8608 (3)	0.0303 (9)
C22	0.1929 (3)	0.5296 (8)	0.6379 (3)	0.0242 (10)
H22A	0.1737	0.5516	0.5694	0.029*
C21	0.2101 (3)	1.1388 (8)	1.0832 (3)	0.0205 (10)
H21A	0.1866	1.2855	1.1085	0.025*
C20	0.2901 (3)	0.6638 (8)	0.8066 (3)	0.0196 (9)
C19	0.0339 (3)	1.1715 (9)	0.9398 (3)	0.0249 (10)
H19A	0.0187	1.3304	0.9575	0.03*
O18	0.3571 (2)	0.4591 (6)	1.2656 (2)	0.0262 (7)
C17	0.1172 (3)	0.8278 (9)	0.9437 (3)	0.0256 (10)
H17A	0.1675	0.6995	0.962	0.031*

supplementary materials

C16	0.7183 (3)	0.3957 (9)	1.5446 (3)	0.0283 (12)
C15	0.2466 (3)	0.4697 (8)	0.8370 (3)	0.0214 (9)
H15A	0.2654	0.4478	0.9054	0.026*
C14	0.5391 (3)	0.3097 (9)	1.4337 (3)	0.0257 (10)
H14A	0.48	0.2064	1.4147	0.031*
C13	0.3831 (3)	1.0697 (8)	1.1102 (3)	0.0194 (9)
H13A	0.4338	1.1726	1.1657	0.023*
C12	0.4342 (3)	0.5834 (8)	1.2935 (3)	0.0209 (10)
C11	0.8179 (3)	0.3260 (12)	1.6335 (3)	0.0429 (14)
H11A	0.8709	0.4508	1.6431	0.064*
H11B	0.8412	0.1632	1.6223	0.064*
H11C	0.8059	0.3188	1.6927	0.064*
C10	0.1487 (3)	0.3368 (9)	0.6677 (3)	0.0245 (10)
C9	0.1769 (3)	0.3097 (9)	0.7689 (3)	0.0261 (10)
H9A	0.1477	0.1794	0.7907	0.031*
C8	0.3638 (3)	0.8416 (9)	0.8767 (3)	0.0220 (9)
C7	0.3513 (3)	0.8494 (8)	1.1542 (3)	0.0180 (9)
H7A	0.3321	0.7032	1.1087	0.022*
C6	0.0724 (3)	0.1619 (9)	0.5931 (3)	0.0337 (12)
H6A	0.0619	0.2086	0.5265	0.051*
H6B	0.0064	0.1713	0.5969	0.051*
H6C	0.0991	−0.0082	0.6075	0.051*
C5	0.6310 (3)	0.2462 (9)	1.5159 (3)	0.0299 (11)
H5A	0.634	0.1001	1.5524	0.036*
C4	0.2640 (3)	0.6893 (9)	0.7056 (3)	0.0266 (10)
H4A	0.295	0.8159	0.6838	0.032*
C3	0.4296 (3)	1.0075 (9)	1.0408 (3)	0.0234 (10)
H3A	0.4392	1.1609	1.0096	0.028*
H3B	0.4979	0.9279	1.0779	0.028*
C2	0.7116 (3)	0.6093 (10)	1.4912 (3)	0.0315 (12)
H2A	0.7703	0.714	1.511	0.038*
C1	0.2577 (3)	0.9476 (9)	1.1657 (3)	0.0199 (9)
H1A	0.2082	0.8122	1.1576	0.024*
H1B	0.2792	1.0256	1.2314	0.024*
O31	0.2904 (2)	1.2143 (5)	1.05768 (19)	0.0208 (7)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O30	0.0189 (14)	0.0291 (16)	0.0216 (15)	−0.0078 (14)	0.0116 (12)	−0.0057 (14)
N29	0.0149 (17)	0.0197 (19)	0.0251 (18)	−0.0006 (16)	0.0087 (15)	−0.0016 (16)
O28	0.0160 (14)	0.0252 (16)	0.0221 (15)	0.0017 (13)	0.0057 (12)	0.0027 (13)
O27	0.0230 (15)	0.0327 (19)	0.0266 (16)	−0.0017 (15)	0.0153 (13)	−0.0005 (15)
C26	0.022 (2)	0.022 (2)	0.020 (2)	0.0020 (19)	0.0131 (18)	−0.0048 (18)
C25	0.023 (2)	0.027 (2)	0.029 (2)	−0.003 (2)	0.010 (2)	−0.001 (2)
C24	0.021 (2)	0.032 (3)	0.029 (2)	0.001 (2)	0.014 (2)	−0.001 (2)
N23	0.0244 (19)	0.033 (2)	0.027 (2)	−0.0011 (19)	0.0055 (17)	0.0014 (19)
C22	0.026 (2)	0.025 (3)	0.022 (2)	0.005 (2)	0.0110 (19)	−0.001 (2)

supplementary materials

C21	0.014 (2)	0.023 (2)	0.027 (2)	−0.0015 (19)	0.0100 (18)	0.001 (2)
C20	0.016 (2)	0.023 (2)	0.022 (2)	0.006 (2)	0.0095 (18)	0.000 (2)
C19	0.017 (2)	0.026 (2)	0.033 (2)	0.007 (2)	0.012 (2)	0.006 (2)
O18	0.0247 (16)	0.0233 (16)	0.0275 (16)	−0.0036 (15)	0.0087 (13)	0.0007 (15)
C17	0.020 (2)	0.028 (2)	0.027 (2)	0.001 (2)	0.009 (2)	−0.001 (2)
C16	0.025 (2)	0.043 (3)	0.019 (2)	0.011 (2)	0.010 (2)	0.001 (2)
C15	0.022 (2)	0.026 (2)	0.018 (2)	0.004 (2)	0.0107 (18)	0.005 (2)
C14	0.026 (2)	0.026 (2)	0.026 (2)	0.004 (2)	0.012 (2)	0.001 (2)
C13	0.016 (2)	0.021 (2)	0.021 (2)	0.0005 (18)	0.0076 (17)	−0.0008 (19)
C12	0.025 (2)	0.018 (2)	0.021 (2)	0.006 (2)	0.0122 (19)	0.002 (2)
C11	0.026 (2)	0.066 (4)	0.034 (3)	0.019 (3)	0.012 (2)	0.010 (3)
C10	0.017 (2)	0.025 (2)	0.028 (2)	0.007 (2)	0.0070 (19)	0.001 (2)
C9	0.021 (2)	0.026 (2)	0.035 (2)	0.005 (2)	0.016 (2)	0.000 (2)
C8	0.018 (2)	0.028 (2)	0.024 (2)	0.006 (2)	0.0132 (19)	0.002 (2)
C7	0.0150 (19)	0.023 (2)	0.017 (2)	−0.0027 (19)	0.0075 (17)	0.0003 (19)
C6	0.024 (2)	0.033 (3)	0.036 (3)	0.001 (2)	0.006 (2)	−0.003 (2)
C5	0.034 (3)	0.035 (3)	0.025 (2)	0.009 (2)	0.017 (2)	0.010 (2)
C4	0.024 (2)	0.033 (3)	0.028 (2)	0.003 (2)	0.016 (2)	0.002 (2)
C3	0.018 (2)	0.029 (3)	0.025 (2)	−0.004 (2)	0.0101 (18)	−0.001 (2)
C2	0.024 (2)	0.044 (3)	0.025 (2)	−0.002 (2)	0.010 (2)	0.000 (2)
C1	0.0130 (19)	0.026 (2)	0.023 (2)	−0.0015 (19)	0.0096 (17)	0.000 (2)
O31	0.0145 (14)	0.0247 (16)	0.0266 (15)	0.0009 (13)	0.0123 (12)	0.0029 (13)

Geometric parameters (Å, °)

O30—C8	1.360 (5)	C16—C2	1.382 (6)
O30—C3	1.450 (5)	C16—C5	1.393 (7)
N29—C19	1.370 (5)	C16—C11	1.516 (6)
N29—C17	1.371 (6)	C15—C9	1.377 (6)
N29—C21	1.462 (5)	C15—H15A	0.95
O28—C12	1.352 (5)	C14—C5	1.400 (6)
O28—C7	1.451 (4)	C14—H14A	0.95
O27—C8	1.220 (5)	C13—O31	1.445 (5)
C26—C14	1.394 (6)	C13—C3	1.509 (5)
C26—C24	1.395 (6)	C13—C7	1.525 (6)
C26—C12	1.480 (5)	C13—H13A	1
C25—C17	1.360 (6)	C11—H11A	0.98
C25—N23	1.379 (6)	C11—H11B	0.98
C25—H25A	0.95	C11—H11C	0.98
C24—C2	1.393 (6)	C10—C9	1.400 (6)
C24—H24A	0.95	C10—C6	1.506 (6)
N23—C19	1.315 (6)	C9—H9A	0.95
C22—C4	1.381 (6)	C7—C1	1.530 (6)
C22—C10	1.393 (6)	C7—H7A	1
C22—H22A	0.95	C6—H6A	0.98
C21—O31	1.432 (5)	C6—H6B	0.98
C21—C1	1.523 (6)	C6—H6C	0.98
C21—H21A	1	C5—H5A	0.95
C20—C15	1.396 (6)	C4—H4A	0.95

supplementary materials

C20—C4	1.404 (5)	C3—H3A	0.99
C20—C8	1.473 (6)	C3—H3B	0.99
C19—H19A	0.95	C2—H2A	0.95
O18—C12	1.205 (5)	C1—H1A	0.99
C17—H17A	0.95	C1—H1B	0.99
C8—O30—C3	116.8 (3)	O28—C12—C26	112.1 (4)
C19—N29—C17	106.3 (3)	C16—C11—H11A	109.5
C19—N29—C21	124.9 (4)	C16—C11—H11B	109.5
C17—N29—C21	128.7 (3)	H11A—C11—H11B	109.5
C12—O28—C7	116.1 (3)	C16—C11—H11C	109.5
C14—C26—C24	118.9 (4)	H11A—C11—H11C	109.5
C14—C26—C12	118.3 (4)	H11B—C11—H11C	109.5
C24—C26—C12	122.7 (4)	C22—C10—C9	118.3 (4)
C17—C25—N23	111.0 (4)	C22—C10—C6	121.0 (4)
C17—C25—H25A	124.5	C9—C10—C6	120.7 (4)
N23—C25—H25A	124.5	C15—C9—C10	120.7 (4)
C2—C24—C26	120.0 (4)	C15—C9—H9A	119.6
C2—C24—H24A	120	C10—C9—H9A	119.6
C26—C24—H24A	120	O27—C8—O30	122.8 (4)
C19—N23—C25	104.4 (4)	O27—C8—C20	125.5 (4)
C4—C22—C10	121.5 (4)	O30—C8—C20	111.7 (4)
C4—C22—H22A	119.2	O28—C7—C13	105.9 (3)
C10—C22—H22A	119.2	O28—C7—C1	114.1 (3)
O31—C21—N29	108.0 (3)	C13—C7—C1	103.3 (3)
O31—C21—C1	106.5 (3)	O28—C7—H7A	111
N29—C21—C1	114.4 (4)	C13—C7—H7A	111
O31—C21—H21A	109.3	C1—C7—H7A	111
N29—C21—H21A	109.3	C10—C6—H6A	109.5
C1—C21—H21A	109.3	C10—C6—H6B	109.5
C15—C20—C4	119.0 (4)	H6A—C6—H6B	109.5
C15—C20—C8	122.6 (4)	C10—C6—H6C	109.5
C4—C20—C8	118.4 (4)	H6A—C6—H6C	109.5
N23—C19—N29	112.3 (4)	H6B—C6—H6C	109.5
N23—C19—H19A	123.8	C16—C5—C14	120.5 (4)
N29—C19—H19A	123.8	C16—C5—H5A	119.8
C25—C17—N29	105.9 (4)	C14—C5—H5A	119.8
C25—C17—H17A	127.1	C22—C4—C20	119.7 (4)
N29—C17—H17A	127.1	C22—C4—H4A	120.2
C2—C16—C5	118.6 (4)	C20—C4—H4A	120.2
C2—C16—C11	121.0 (5)	O30—C3—C13	108.4 (3)
C5—C16—C11	120.3 (4)	O30—C3—H3A	110
C9—C15—C20	120.7 (4)	C13—C3—H3A	110
C9—C15—H15A	119.6	O30—C3—H3B	110
C20—C15—H15A	119.6	C13—C3—H3B	110
C26—C14—C5	120.4 (4)	H3A—C3—H3B	108.4
C26—C14—H14A	119.8	C16—C2—C24	121.5 (5)
C5—C14—H14A	119.8	C16—C2—H2A	119.2
O31—C13—C3	109.2 (3)	C24—C2—H2A	119.2
O31—C13—C7	105.8 (3)	C21—C1—C7	104.1 (3)

C3—C13—C7	116.1 (4)	C21—C1—H1A	110.9
O31—C13—H13A	108.5	C7—C1—H1A	110.9
C3—C13—H13A	108.5	C21—C1—H1B	110.9
C7—C13—H13A	108.5	C7—C1—H1B	110.9
O18—C12—O28	123.0 (4)	H1A—C1—H1B	109
O18—C12—C26	124.9 (4)	C21—O31—C13	111.3 (3)
C12—O28—C7—C1	75.4 (5)	C22—C4—C20—C8	−178.2 (4)
C12—O28—C7—C13	−171.7 (3)	C22—C4—C20—C15	2.7 (7)
C7—O28—C12—O18	−7.0 (6)	C20—C4—C22—C10	−2.3 (7)
C7—O28—C12—C26	171.5 (3)	C14—C5—C16—C2	1.0 (7)
C8—O30—C3—C13	153.6 (4)	C14—C5—C16—C11	−179.8 (4)
C3—O30—C8—O27	−1.7 (6)	C16—C5—C14—C26	0.0 (7)
C3—O30—C8—C20	180.0 (4)	O28—C7—C13—O31	−146.7 (3)
C21—O31—C13—C3	139.0 (4)	O28—C7—C13—C3	92.0 (4)
C21—O31—C13—C7	13.4 (4)	C1—C7—C13—O31	−26.5 (4)
C13—O31—C21—N29	−117.7 (3)	C1—C7—C13—C3	−147.8 (4)
C13—O31—C21—C1	5.6 (4)	O30—C8—C20—C15	−17.9 (6)
C19—N23—C25—C17	1.3 (5)	O27—C8—C20—C15	163.9 (5)
C25—N23—C19—N29	−1.3 (5)	O30—C8—C20—C4	163.0 (4)
C19—N29—C17—C25	0.0 (5)	O27—C8—C20—C4	−15.2 (7)
C19—N29—C21—O31	−104.2 (4)	C15—C9—C10—C6	−180.0 (4)
C19—N29—C21—C1	137.4 (4)	C10—C9—C15—C20	0.5 (7)
C21—N29—C19—N23	177.9 (4)	C15—C9—C10—C22	0.0 (7)
C21—N29—C17—C25	−176.9 (4)	C6—C10—C22—C4	−179.1 (4)
C17—N29—C19—N23	0.9 (5)	C9—C10—C22—C4	1.0 (7)
C17—N29—C21—O31	72.1 (5)	O18—C12—C26—C24	−179.6 (4)
C17—N29—C21—C1	−46.3 (6)	O28—C12—C26—C14	−179.6 (4)
C21—C1—C7—C13	29.4 (4)	O18—C12—C26—C14	−1.1 (7)
C7—C1—C21—O31	−22.1 (4)	O28—C12—C26—C24	1.9 (6)
C21—C1—C7—O28	143.8 (4)	C5—C14—C26—C12	−179.5 (4)
C7—C1—C21—N29	97.1 (4)	C5—C14—C26—C24	−0.9 (7)
C16—C2—C24—C26	0.2 (7)	C9—C15—C20—C8	179.1 (4)
C24—C2—C16—C11	179.7 (4)	C9—C15—C20—C4	−1.8 (7)
C24—C2—C16—C5	−1.1 (7)	N29—C17—C25—N23	−0.8 (5)
O30—C3—C13—O31	−67.2 (4)	C2—C24—C26—C14	0.8 (7)
O30—C3—C13—C7	52.4 (5)	C2—C24—C26—C12	179.3 (4)

Fig. 1

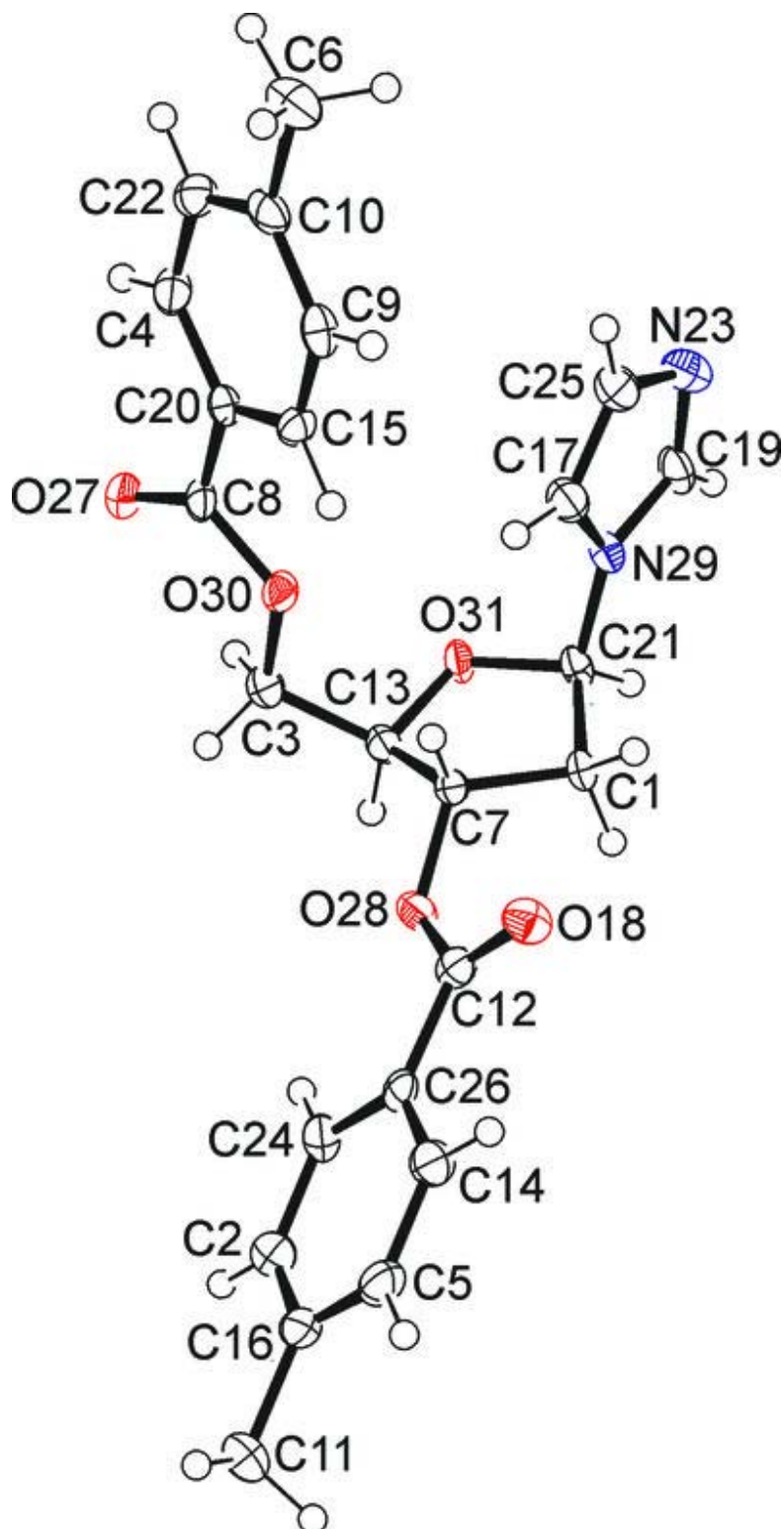


Fig. 2

