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Euphorbia factor L_8: a diterpenoid from the seeds of *Euphorbia lathyris*

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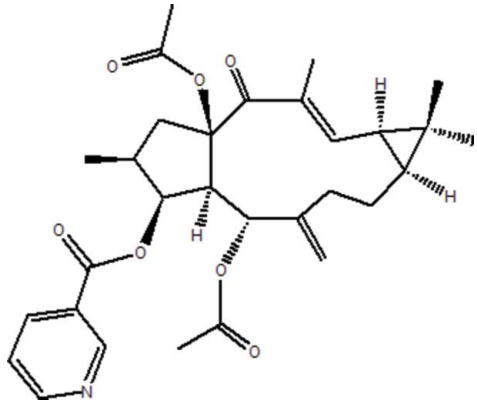
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.049; wR factor = 0.118; data-to-parameter ratio = 8.7.

The title compound [systematic name: (2*S**,3*S**,4*R**,5*R**,9*S**,11*S**,15*R**)-5,15-diacetoxy-3-nicotinoyloxy-14-oxolathyra-6(17),12(*E*)-diene], $C_{30}H_{37}NO_7$, was isolated from the seeds of *Euphorbia lathyris*. The tricyclic diterpenoid molecule contains an 11-membered ring, a five-membered ring exhibiting an envelope conformation and a three-membered ring. The 11-membered ring is *cis*-fused with the three-membered ring and *trans*-fused with the five-membered ring.

Related literature

For related literature, see: Appendino *et al.* (1999); Fujiwara *et al.* (1996); Kupchan *et al.* (1976); the Pharmacopoeia Commission of the People's Republic of China (2005).



Experimental

Crystal data

$C_{30}H_{37}NO_7$
M_r = 523.61
Orthorhombic, $P2_12_12_1$
a = 10.162 (6) Å
b = 15.249 (5) Å
c = 18.802 (9) Å
V = 2914 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.36 × 0.34 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3444 measured reflections
3065 independent reflections
1462 reflections with $I > 2\sigma(I)$
R_{int} = 0.003
3 standard reflections
every 300 reflections
intensity decay: 0.3%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.118
S = 0.93
3065 reflections
354 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *DIFRAC* (Gabe & White, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2099).

References

Appendino, G., Tron, G. C., Cravotto, G., Palmisano, G. & Jakupovic, J. (1999). *J. Nat. Prod.* **62**, 76–79.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Fujiwara, M., Ijichi, K., Tokuhisa, K., Katsuura, K., Shigeta, S., Konno, K., Wang, G.-Y.-S., Uemura, D., Yokota, T. & Baba, M. (1996). *Antimicrob. Agents Chemother.* **40**, 271–273.
Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.
Gabe, E. J. & White, P. S. (1993). *DIFRAC. Am. Crystallogr. Assoc. Meet.*, Pittsburgh, Abstract PA 104.
Kupchan, S. M., Uchida, I., Branfman, A. R., Dailey, R. G. Jr & Fel, B. Y. (1976). *Science*, **191**, 571–572.
Pharmacopoeia Commission of the People's Republic of China (2005). *Pharmacopoeia of the People's Republic of China 2005*, p. 24. Beijing: Chemical Industry Press.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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Euphorbia factor L_8: a diterpenoid from the seeds of *Euphorbia lathyris*

Wei Jiao, Zhi-hua Mao, Wei-wei Dong, Mei-cai Deng and Run-hua Lu

S1. Comment

The seed of *Euphorbia lathyris* is a traditional Chinese medicine which has been used for the treatment of hydropsy, ascites, amenorrhea, scabies (Pharmacopoeia Commission of the People's Republic of China, 2005). Several constituents in this plant proved to have significant activity (Kupchan *et al.*, 1976; Fujiwara *et al.*, 1996) and this medicine has been used to treat tumors and cancer in many countries. In our current investigation, *Euphorbia* Factor L_8 (I) was isolated from the seeds of this plant. The structure of (I) was elucidated by comprehensive spectroscopic analysis, and was confirmed by single-crystal X-ray diffraction analysis reported here (Fig. 1). The title compound shows the tricyclic terpenoid skeleton of lathyrane, consisting of fused five-, eleven- and three-membered rings (A: C1–C4/C15, B: C4–C9/C11–C15, C: C9–C11). Rings A and B are *trans*-joined (torsion angle H4–C4–C15–O3 = -152.8°), while rings B and C are *cis*-joined (H9–C9–C11–H11 = 0.99°). Ring A adopts an envelope conformation, with atom C3 0.64 Å out of the plane defined by atoms C1/C2/C4/C15.

S2. Experimental

The seeds of *E. lathyris* (10 kg) were collected in Sichuan province, People's Republic of China and extracted with 95% EtOH at room temperature. The extract was concentrated *in vacuo* and filtered. The filtrate was partitioned between EtOAc and H_2O. The EtOAc soluble materials (1 kg) were subjected to silica-gel column chromatography (160–200 mesh, 4 kg) with petrol-EtOAc stepwise elution. The column chromatographic fractions (500 ml each) were combined into 12 fractions according to thin-layer chromatography monitoring analysis. Fraction 5 (7.5 g) was applied to a RP-18 silica-gel column and eluted with MeOH/H_2O (7:3) to yield five fractions. Fraction 5.2 (1.4 g) was subjected to silica-gel column chromatography (200–300 mesh, 50 g) and eluted with petrol-EtOAc (5:1) to afford the compound (I). The isolated product was recrystallized at room temperature from acetone to afford the block crytals. ^{13}C NMR (150 MHz, $CDCl_3$, δ, p.p.m.): 48.6(C1), 37.7(C2), 81.6(C3), 52.3(C4), 65.5(C5), 144.4(C6), 34.9(C7), 21.0(C8), 35.4(C9), 25.3(C10), 28.5(C11), 146.6(C12), 134.3(C13), 196.6(C14), 92.5(C15), 14.2(C16), 115.5(C17), 29.0(C18), 16.8(C19), 12.4(C20), 164.9(C21), 126.0(C22), 137.0(C23), 123.3(C24), 153.5(C25), 151.0(C26), 170.2(C27), 21.6(C28), 169.7(C29), 22.1(C30).

S3. Refinement

All hydrogen atoms were located geometrically with C—H distances of 0.93–0.98 Å, and refined using a riding model. The absolute configuration could not be determined from the X-ray analysis, owing to the absence of strong anomalous scatterers, and Friedel pairs were averaged. However, the absolute configuration can be suggested on a biogenetic basis (Appendino *et al.*, 1999).

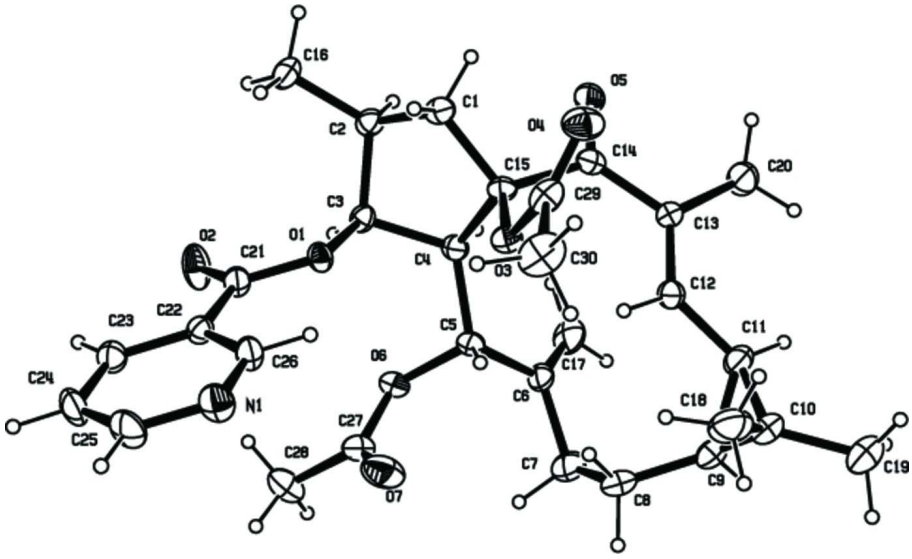

Figure 1

ORTEP plot of compound (I) showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

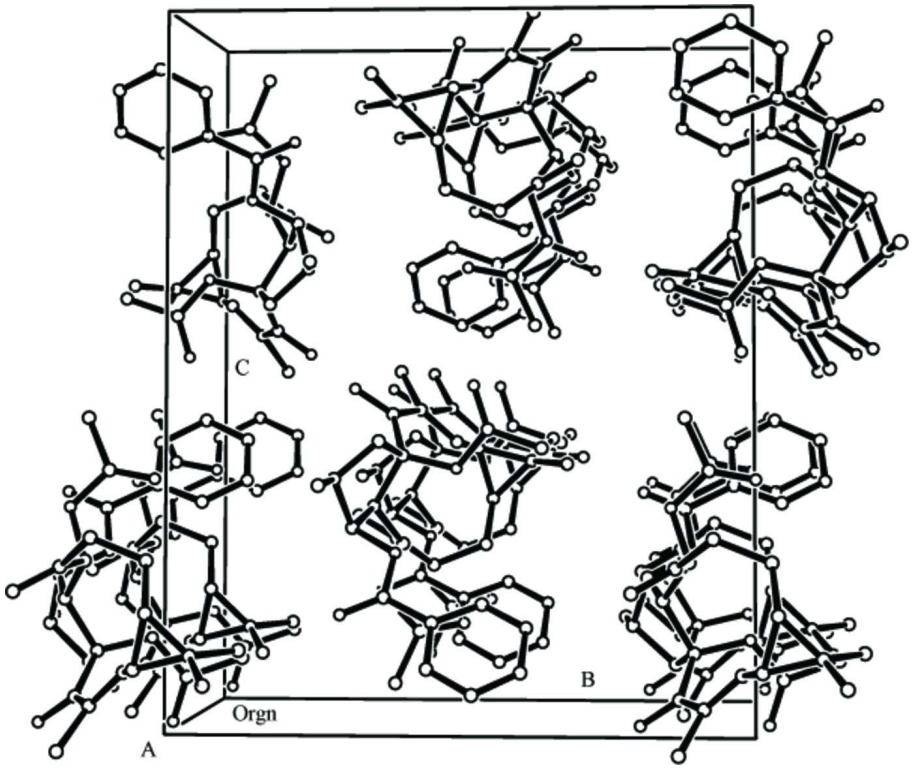

Figure 2

The crystal packing of (I), viewed down the *a* axis. H-atoms omitted for clarity.

(2*S,3*S**,4*R**,5*R**,9*S**,11*S**, 15*R**)-5,15-diacetoxy-3-nicotinoyloxy-14-oxolathyra-6(17),12(*E*)- diene**

Crystal data

$C_{30}H_{37}NO_7$
$M_r = 523.61$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 10.162$ (6) Å
$b = 15.249$ (5) Å
$c = 18.802$ (9) Å
$V = 2914$ (2) Å^3
$Z = 4$
$F(000) = 1120$
$D_x = 1.194$ Mg m^{-3}
Melting point: 469(1) K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 24 reflections
$\theta = 4.5$–$5.5°$
$\mu = 0.08$ mm^{-1}
$T = 298$ K
Block, colourless
0.36 × 0.34 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
3444 measured reflections
3065 independent reflections
1462 reflections with $I > 2\sigma(I)$
$R_{int} = 0.003$
$\theta_{max} = 25.5°$, $\theta_{min} = 1.7°$
$h = -1 \rightarrow 12$
$k = -3 \rightarrow 18$
$l = -1 \rightarrow 22$
3 standard reflections every 300 reflections
intensity decay: 0.3%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.118$
$S = 0.93$
3065 reflections
354 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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	0.4410 (3)	0.60363 (17)	0.75057 (16)	0.0422 (8)
O2	0.3383 (4)	0.6889 (2)	0.67028 (18)	0.0745 (12)
O3	0.6027 (3)	0.50915 (17)	0.86366 (15)	0.0442 (8)
O4	0.5648 (4)	0.4774 (2)	0.97859 (19)	0.0725 (11)

O5	0.6858 (4)	0.6902 (2)	0.97413 (16)	0.0600 (10)
O6	0.6894 (4)	0.63864 (19)	0.68532 (16)	0.0539 (9)
O7	0.6709 (5)	0.4992 (3)	0.6477 (2)	0.0887 (14)
N1	0.3198 (5)	0.3782 (2)	0.6543 (2)	0.0653 (13)
C1	0.4680 (5)	0.6336 (3)	0.9021 (2)	0.0463 (13)
H1A	0.4056	0.5857	0.8985	0.071 (7)*
H1B	0.4675	0.6552	0.9506	0.071 (7)*
C2	0.4308 (5)	0.7065 (3)	0.8509 (2)	0.0465 (12)
H2	0.4703	0.7610	0.8684	0.045 (5)*
C3	0.5024 (5)	0.6806 (3)	0.7833 (2)	0.0401 (12)
H3	0.5082	0.7297	0.7498	0.045 (5)*
C4	0.6377 (5)	0.6534 (3)	0.8103 (2)	0.0405 (12)
H4	0.6821	0.7076	0.8246	0.045 (5)*
C5	0.7290 (5)	0.6088 (3)	0.7565 (2)	0.0441 (12)
H5	0.7175	0.5451	0.7596	0.045 (5)*
C6	0.8749 (5)	0.6304 (3)	0.7607 (3)	0.0491 (14)
C7	0.9639 (6)	0.5689 (4)	0.7203 (3)	0.0763 (18)
H7A	1.0510	0.5950	0.7184	0.071 (7)*
H7B	0.9318	0.5648	0.6718	0.071 (7)*
C8	0.9773 (6)	0.4764 (4)	0.7498 (3)	0.0732 (17)
H8A	0.8901	0.4547	0.7612	0.071 (7)*
H8B	1.0129	0.4391	0.7127	0.071 (7)*
C9	1.0623 (6)	0.4677 (4)	0.8146 (3)	0.0686 (15)
H9	1.1538	0.4847	0.8055	0.045 (5)*
C10	1.0512 (6)	0.3977 (4)	0.8693 (3)	0.0697 (17)
C11	1.0173 (5)	0.4919 (3)	0.8887 (3)	0.0586 (16)
H11	1.0834	0.5220	0.9178	0.045 (5)*
C12	0.8824 (5)	0.5235 (3)	0.8982 (2)	0.0454 (12)
H12	0.8184	0.4984	0.8693	0.064 (7)*
C13	0.8419 (5)	0.5850 (3)	0.9442 (2)	0.0446 (12)
C14	0.7110 (5)	0.6257 (3)	0.9385 (2)	0.0443 (12)
C15	0.6070 (5)	0.6020 (3)	0.8815 (2)	0.0410 (12)
C16	0.2825 (5)	0.7213 (3)	0.8442 (3)	0.0612 (15)
H16A	0.2414	0.6687	0.8271	0.129 (6)*
H16B	0.2661	0.7683	0.8115	0.129 (6)*
H16C	0.2468	0.7361	0.8899	0.129 (6)*
C17	0.9201 (6)	0.7006 (4)	0.7918 (3)	0.0720 (16)
H17A	1.0093	0.7138	0.7894	0.089 (15)*
H17B	0.8631	0.7374	0.8164	0.089 (15)*
C18	0.9437 (7)	0.3300 (4)	0.8661 (3)	0.090 (2)
H18A	0.9760	0.2784	0.8426	0.129 (6)*
H18B	0.8702	0.3532	0.8401	0.129 (6)*
H18C	0.9164	0.3153	0.9134	0.129 (6)*
C19	1.1778 (7)	0.3627 (5)	0.9013 (4)	0.112 (3)
H19A	1.2163	0.3207	0.8694	0.129 (6)*
H19B	1.1591	0.3350	0.9460	0.129 (6)*
H19C	1.2382	0.4102	0.9086	0.129 (6)*
C20	0.9313 (6)	0.6255 (3)	0.9990 (3)	0.0698 (16)

H20A	0.9596	0.6822	0.9829	0.129 (6)*
H20B	1.0067	0.5885	1.0059	0.129 (6)*
H20C	0.8847	0.6316	1.0431	0.129 (6)*
C21	0.3664 (5)	0.6179 (3)	0.6929 (3)	0.0453 (12)
C22	0.3204 (5)	0.5350 (3)	0.6607 (2)	0.0411 (12)
C23	0.2381 (5)	0.5386 (3)	0.6026 (3)	0.0531 (13)
H23	0.2099	0.5925	0.5852	0.064 (7)*
C24	0.1981 (6)	0.4628 (4)	0.5708 (3)	0.0655 (15)
H24	0.1428	0.4639	0.5314	0.064 (7)*
C25	0.2414 (6)	0.3849 (4)	0.5984 (3)	0.0697 (17)
H25	0.2141	0.3334	0.5764	0.064 (7)*
C26	0.3572 (5)	0.4531 (3)	0.6841 (3)	0.0511 (13)
H26	0.4121	0.4500	0.7236	0.064 (7)*
C27	0.6664 (6)	0.5762 (4)	0.6360 (3)	0.0630 (16)
C28	0.6346 (7)	0.6157 (4)	0.5654 (2)	0.089 (2)
H28A	0.6076	0.5703	0.5332	0.129 (6)*
H28B	0.7111	0.6447	0.5469	0.129 (6)*
H28C	0.5646	0.6575	0.5709	0.129 (6)*
C29	0.5746 (5)	0.4539 (3)	0.9179 (3)	0.0548 (13)
C30	0.5620 (7)	0.3613 (3)	0.8920 (4)	0.085 (2)
H30A	0.5472	0.3230	0.9318	0.129 (6)*
H30B	0.6414	0.3444	0.8681	0.129 (6)*
H30C	0.4891	0.3572	0.8597	0.129 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.043 (2)	0.0396 (17)	0.0435 (17)	−0.0049 (17)	−0.0102 (19)	−0.0047 (16)
O2	0.093 (3)	0.0434 (18)	0.088 (3)	−0.003 (2)	−0.046 (3)	0.0091 (19)
O3	0.046 (2)	0.0370 (17)	0.0495 (18)	−0.0018 (16)	0.0047 (19)	−0.0033 (15)
O4	0.087 (3)	0.067 (2)	0.063 (2)	0.003 (2)	0.026 (3)	0.013 (2)
O5	0.070 (3)	0.0543 (18)	0.0553 (18)	0.013 (2)	−0.012 (2)	−0.0226 (17)
O6	0.059 (2)	0.065 (2)	0.0376 (17)	0.0056 (19)	0.004 (2)	−0.0063 (17)
O7	0.119 (4)	0.076 (3)	0.072 (2)	0.003 (3)	0.004 (3)	−0.026 (2)
N1	0.080 (4)	0.044 (2)	0.072 (3)	0.000 (3)	−0.014 (3)	−0.010 (2)
C1	0.043 (3)	0.046 (3)	0.050 (3)	−0.001 (2)	0.006 (3)	−0.006 (2)
C2	0.042 (3)	0.044 (3)	0.054 (3)	0.001 (3)	0.000 (3)	−0.010 (2)
C3	0.032 (3)	0.040 (3)	0.049 (3)	−0.003 (2)	−0.002 (3)	−0.001 (2)
C4	0.037 (3)	0.044 (2)	0.040 (2)	−0.007 (2)	0.001 (3)	−0.005 (2)
C5	0.046 (3)	0.052 (3)	0.034 (3)	0.002 (3)	0.007 (3)	0.001 (2)
C6	0.036 (3)	0.068 (3)	0.044 (3)	0.003 (3)	0.004 (3)	0.008 (3)
C7	0.055 (4)	0.107 (5)	0.067 (4)	0.016 (4)	0.019 (4)	0.004 (4)
C8	0.061 (4)	0.094 (4)	0.065 (3)	0.024 (4)	0.013 (4)	−0.018 (3)
C9	0.038 (3)	0.096 (4)	0.072 (4)	0.016 (4)	0.006 (3)	−0.008 (4)
C10	0.056 (4)	0.079 (4)	0.074 (4)	0.026 (4)	0.002 (4)	−0.009 (3)
C11	0.042 (4)	0.067 (4)	0.067 (3)	0.011 (3)	−0.005 (3)	−0.016 (3)
C12	0.039 (3)	0.052 (3)	0.046 (3)	−0.004 (3)	−0.003 (3)	−0.005 (2)
C13	0.042 (3)	0.050 (3)	0.042 (3)	0.008 (3)	0.001 (3)	−0.004 (2)

C14	0.052 (4)	0.043 (3)	0.037 (3)	0.001 (3)	0.004 (3)	−0.002 (3)
C15	0.046 (3)	0.035 (2)	0.042 (3)	0.000 (2)	0.004 (3)	−0.007 (2)
C16	0.037 (3)	0.075 (3)	0.072 (4)	0.010 (3)	−0.002 (3)	−0.007 (3)
C17	0.036 (4)	0.097 (4)	0.082 (4)	−0.013 (4)	0.006 (4)	0.011 (4)
C18	0.098 (5)	0.074 (4)	0.097 (4)	0.020 (4)	0.012 (5)	−0.023 (3)
C19	0.092 (6)	0.132 (6)	0.111 (5)	0.060 (5)	−0.011 (5)	−0.021 (5)
C20	0.061 (4)	0.073 (3)	0.075 (3)	0.006 (3)	−0.017 (4)	−0.026 (3)
C21	0.046 (3)	0.042 (3)	0.048 (3)	0.002 (3)	−0.008 (3)	−0.002 (3)
C22	0.039 (3)	0.039 (2)	0.046 (3)	0.002 (3)	−0.002 (3)	−0.002 (2)
C23	0.053 (4)	0.053 (3)	0.053 (3)	0.004 (3)	−0.006 (3)	0.000 (3)
C24	0.073 (4)	0.071 (3)	0.053 (3)	0.002 (4)	−0.029 (3)	−0.014 (3)
C25	0.082 (5)	0.058 (4)	0.069 (3)	−0.015 (4)	−0.016 (4)	−0.025 (3)
C26	0.051 (3)	0.050 (3)	0.052 (3)	0.000 (3)	−0.014 (3)	−0.002 (2)
C27	0.058 (4)	0.079 (4)	0.052 (3)	0.009 (4)	0.007 (3)	−0.016 (3)
C28	0.104 (5)	0.117 (5)	0.045 (3)	0.003 (5)	−0.004 (4)	−0.006 (3)
C29	0.044 (3)	0.044 (3)	0.077 (4)	−0.004 (3)	0.007 (3)	0.007 (3)
C30	0.085 (5)	0.045 (3)	0.126 (5)	−0.011 (4)	0.011 (5)	−0.004 (3)

Geometric parameters (Å, º)

O1—C21	1.340 (5)	C10—C11	1.522 (7)
O1—C3	1.465 (5)	C11—C12	1.463 (7)
O2—C21	1.198 (5)	C11—H11	0.9800
O3—C29	1.354 (6)	C12—C13	1.341 (6)
O3—C15	1.457 (5)	C12—H12	0.9300
O4—C29	1.199 (6)	C13—C14	1.471 (7)
O5—C14	1.217 (5)	C13—C20	1.507 (7)
O6—C27	1.349 (6)	C14—C15	1.547 (6)
O6—C5	1.470 (5)	C16—H16A	0.9600
O7—C27	1.196 (6)	C16—H16B	0.9600
N1—C25	1.323 (6)	C16—H16C	0.9600
N1—C26	1.328 (5)	C17—H17A	0.9300
C1—C2	1.518 (6)	C17—H17B	0.9300
C1—C15	1.542 (6)	C18—H18A	0.9600
C1—H1A	0.9700	C18—H18B	0.9600
C1—H1B	0.9700	C18—H18C	0.9600
C2—C3	1.516 (6)	C19—H19A	0.9600
C2—C16	1.529 (7)	C19—H19B	0.9600
C2—H2	0.9800	C19—H19C	0.9600
C3—C4	1.523 (6)	C20—H20A	0.9600
C3—H3	0.9800	C20—H20B	0.9600
C4—C5	1.532 (6)	C20—H20C	0.9600
C4—C15	1.582 (6)	C21—C22	1.478 (6)
C4—H4	0.9800	C22—C26	1.375 (6)
C5—C6	1.521 (7)	C22—C23	1.377 (6)
C5—H5	0.9800	C23—C24	1.364 (6)
C6—C17	1.303 (7)	C23—H23	0.9300
C6—C7	1.508 (7)	C24—C25	1.368 (7)

C7—C8	1.521 (7)	C24—H24	0.9300
C7—H7A	0.9700	C25—H25	0.9300
C7—H7B	0.9700	C26—H26	0.9300
C8—C9	1.500 (7)	C27—C28	1.492 (7)
C8—H8A	0.9700	C28—H28A	0.9600
C8—H8B	0.9700	C28—H28B	0.9600
C9—C10	1.487 (7)	C28—H28C	0.9600
C9—C11	1.513 (7)	C29—C30	1.499 (7)
C9—H9	0.9800	C30—H30A	0.9600
C10—C18	1.504 (8)	C30—H30B	0.9600
C10—C19	1.518 (8)	C30—H30C	0.9600

C21—O1—C3	116.8 (3)	O5—C14—C13	119.4 (5)
C29—O3—C15	115.9 (3)	O5—C14—C15	115.2 (4)
C27—O6—C5	117.0 (4)	C13—C14—C15	124.7 (4)
C25—N1—C26	116.1 (4)	O3—C15—C1	109.5 (4)
C2—C1—C15	107.4 (4)	O3—C15—C14	114.0 (4)
C2—C1—H1A	110.2	C1—C15—C14	112.4 (4)
C15—C1—H1A	110.2	O3—C15—C4	106.9 (3)
C2—C1—H1B	110.2	C1—C15—C4	103.7 (4)
C15—C1—H1B	110.2	C14—C15—C4	109.6 (4)
H1A—C1—H1B	108.5	C2—C16—H16A	109.5
C3—C2—C1	102.8 (3)	C2—C16—H16B	109.5
C3—C2—C16	116.3 (4)	H16A—C16—H16B	109.5
C1—C2—C16	113.9 (4)	C2—C16—H16C	109.5
C3—C2—H2	107.8	H16A—C16—H16C	109.5
C1—C2—H2	107.8	H16B—C16—H16C	109.5
C16—C2—H2	107.8	C6—C17—H17A	120.0
O1—C3—C2	110.9 (4)	C6—C17—H17B	120.0
O1—C3—C4	107.8 (3)	H17A—C17—H17B	120.0
C2—C3—C4	103.0 (4)	C10—C18—H18A	109.5
O1—C3—H3	111.6	C10—C18—H18B	109.5
C2—C3—H3	111.6	H18A—C18—H18B	109.5
C4—C3—H3	111.6	C10—C18—H18C	109.5
C3—C4—C5	116.6 (4)	H18A—C18—H18C	109.5
C3—C4—C15	103.8 (4)	H18B—C18—H18C	109.5
C5—C4—C15	117.3 (4)	C10—C19—H19A	109.5
C3—C4—H4	106.1	C10—C19—H19B	109.5
C5—C4—H4	106.1	H19A—C19—H19B	109.5
C15—C4—H4	106.1	C10—C19—H19C	109.5
O6—C5—C6	104.4 (4)	H19A—C19—H19C	109.5
O6—C5—C4	107.3 (4)	H19B—C19—H19C	109.5
C6—C5—C4	117.4 (4)	C13—C20—H20A	109.5
O6—C5—H5	109.2	C13—C20—H20B	109.5
C6—C5—H5	109.2	H20A—C20—H20B	109.5
C4—C5—H5	109.2	C13—C20—H20C	109.5
C17—C6—C7	121.7 (5)	H20A—C20—H20C	109.5
C17—C6—C5	123.0 (5)	H20B—C20—H20C	109.5

C7—C6—C5	115.1 (5)	O2—C21—O1	124.7 (4)
C6—C7—C8	116.5 (4)	O2—C21—C22	123.5 (4)
C6—C7—H7A	108.2	O1—C21—C22	111.8 (4)
C8—C7—H7A	108.2	C26—C22—C23	117.1 (4)
C6—C7—H7B	108.2	C26—C22—C21	124.0 (4)
C8—C7—H7B	108.2	C23—C22—C21	118.8 (4)
H7A—C7—H7B	107.3	C24—C23—C22	119.6 (5)
C9—C8—C7	115.4 (5)	C24—C23—H23	120.2
C9—C8—H8A	108.4	C22—C23—H23	120.2
C7—C8—H8A	108.4	C23—C24—C25	118.3 (5)
C9—C8—H8B	108.4	C23—C24—H24	120.9
C7—C8—H8B	108.4	C25—C24—H24	120.9
H8A—C8—H8B	107.5	N1—C25—C24	124.2 (5)
C10—C9—C8	125.6 (5)	N1—C25—H25	117.9
C10—C9—C11	61.0 (3)	C24—C25—H25	117.9
C8—C9—C11	123.5 (5)	N1—C26—C22	124.6 (4)
C10—C9—H9	112.5	N1—C26—H26	117.7
C8—C9—H9	112.5	C22—C26—H26	117.7
C11—C9—H9	112.5	O7—C27—O6	124.0 (5)
C9—C10—C18	121.3 (5)	O7—C27—C28	124.7 (5)
C9—C10—C19	117.5 (6)	O6—C27—C28	111.4 (5)
C18—C10—C19	113.0 (5)	C27—C28—H28A	109.5
C9—C10—C11	60.4 (4)	C27—C28—H28B	109.5
C18—C10—C11	119.6 (5)	H28A—C28—H28B	109.5
C19—C10—C11	115.4 (5)	C27—C28—H28C	109.5
C12—C11—C9	118.4 (5)	H28A—C28—H28C	109.5
C12—C11—C10	123.5 (5)	H28B—C28—H28C	109.5
C9—C11—C10	58.7 (3)	O4—C29—O3	123.3 (4)
C12—C11—H11	114.9	O4—C29—C30	125.7 (5)
C9—C11—H11	114.9	O3—C29—C30	111.0 (5)
C10—C11—H11	114.9	C29—C30—H30A	109.5
C13—C12—C11	126.6 (5)	C29—C30—H30B	109.5
C13—C12—H12	116.7	H30A—C30—H30B	109.5
C11—C12—H12	116.7	C29—C30—H30C	109.5
C12—C13—C14	121.7 (4)	H30A—C30—H30C	109.5
C12—C13—C20	122.9 (5)	H30B—C30—H30C	109.5
C14—C13—C20	115.0 (4)		