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24(*R*)-Acetyloxy-1α,2α-epoxycholesta-4,6-dien-3-one hydrate. Erratum

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In the paper by Rajalakshmi *et al*. [*Acta Cryst.* (2000), C**56**, e307–308], it is incorrectly stated that 'the priority sequence attached to the chiral carbon C24 has an '*R*' designation as per the listed coordinates'. This is corrected as 'the priority sequence attached to the chiral carbon C24 has an '*S*' designation as per the listed coordinates'.

supporting information

Acta Cryst. (2000). C**56**, e538 [https://doi.org/10.1107/S0108270100012993]

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Computing details

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *SHELXL* and *PARST* (Nardelli, 1983).

1a,2a-Epoxy-24(*R*)-acyloxycholesta-4,6-dien-3-one hydrate

Crystal data

$C_{29}H_{42}O_4 \cdot H_2O$
$M_r = 472.64$
Monoclinic, $P2_1$
$a = 10.642$ (3) Å
$b = 11.719$ (2) Å
$c = 10.977$ (3) Å
$\beta = 108.04$ (2)°
$V = 1301.7$ (6) Å^3
$Z = 2$
$F(000) = 512$
$D_x = 1.206$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å
Cell parameters from 25 reflections
$\theta = 10$–27°
$\mu = 0.64$ mm^{-1}
$T = 293$ K
Rectangle, colourless
0.20 × 0.15 × 0.10 mm

Data collection

Enraf-Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
2848 measured reflections
2712 independent reflections
2262 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 74.9°$, $\theta_{min} = 4.2°$
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 13$
$l = -13 \rightarrow 13$
3 standard reflections every 120 min
intensity decay: <3%

Refinement

Refinement on F^2
Least-squares matrix: full with fixed elements per cycle
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.162$
$S = 1.12$
2712 reflections
322 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
Calculated $w = 1/[\sigma^2(F_o^2) + (0.095P)^2 + 0.2101P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.010$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.55$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0091 (15)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.0854 (3)	1.8844 (3)	0.0756 (3)	0.0670 (9)
O2	−0.1021 (3)	1.5957 (3)	0.1111 (3)	0.0555 (7)
O3	0.3554 (2)	0.8864 (3)	0.9399 (2)	0.0453 (6)
O4	0.1624 (3)	0.8141 (3)	0.9464 (3)	0.0678 (9)
C1	0.0359 (4)	1.5926 (4)	0.1243 (3)	0.0478 (9)
H1	0.0610	1.5387	0.0677	0.057*
C2	−0.0438 (4)	1.6889 (4)	0.0602 (4)	0.0506 (9)
H2	−0.0648	1.6938	−0.0331	0.061*
C3	−0.0375 (4)	1.7967 (4)	0.1312 (4)	0.0477 (9)
C4	0.0241 (4)	1.7899 (4)	0.2703 (4)	0.0494 (9)
H4	0.0130	1.8512	0.3199	0.059*
C5	0.0952 (4)	1.7006 (4)	0.3300 (3)	0.0433 (8)
C6	0.1415 (5)	1.6968 (4)	0.4687 (4)	0.0559 (11)
H6	0.1273	1.7602	0.5137	0.067*
C7	0.2039 (5)	1.6063 (4)	0.5356 (4)	0.0537 (10)
H7	0.2307	1.6095	0.6246	0.064*
C8	0.2314 (4)	1.5016 (4)	0.4727 (3)	0.0438 (8)
H8	0.3211	1.5083	0.4668	0.053*
C9	0.1357 (4)	1.4910 (3)	0.3352 (3)	0.0390 (8)
H9	0.0470	1.4828	0.3434	0.047*
C10	0.1339 (3)	1.6025 (4)	0.2590 (3)	0.0410 (8)
C11	0.1616 (5)	1.3822 (4)	0.2691 (3)	0.0524 (10)
H11A	0.0927	1.3740	0.1876	0.063*
H11B	0.2451	1.3902	0.2517	0.063*
C12	0.1660 (5)	1.2753 (4)	0.3478 (3)	0.0519 (10)
H12A	0.1909	1.2111	0.3043	0.062*
H12B	0.0783	1.2602	0.3533	0.062*
C13	0.2639 (4)	1.2843 (3)	0.4842 (3)	0.0408 (8)
C14	0.2250 (4)	1.3914 (4)	0.5447 (3)	0.0424 (8)
H14	0.1320	1.3813	0.5394	0.051*
C15	0.3035 (5)	1.3823 (4)	0.6861 (4)	0.0582 (11)
H15A	0.3913	1.4142	0.7027	0.070*
H15B	0.2589	1.4218	0.7386	0.070*
C16	0.3102 (5)	1.2547 (4)	0.7126 (3)	0.0537 (11)
H16A	0.2593	1.2358	0.7695	0.064*

H16B	0.4011	1.2314	0.7531	0.064*
C17	0.2524 (4)	1.1927 (4)	0.5825 (3)	0.0436 (8)
H17	0.1579	1.1820	0.5698	0.052*
C18	0.4057 (4)	1.2893 (5)	0.4795 (5)	0.0609 (12)
H18A	0.4243	1.2217	0.4389	0.091*
H18B	0.4656	1.2942	0.5650	0.091*
H18C	0.4162	1.3552	0.4315	0.091*
C19	0.2694 (4)	1.6302 (4)	0.2444 (5)	0.0599 (12)
H19A	0.2957	1.5696	0.1987	0.090*
H19B	0.3334	1.6381	0.3276	0.090*
H19C	0.2639	1.7003	0.1977	0.090*
C20	0.3119 (4)	1.0738 (4)	0.5832 (3)	0.0463 (9)
H20	0.4079	1.0833	0.6065	0.056*
C21	0.2671 (6)	1.0148 (5)	0.4531 (4)	0.0696 (14)
H21A	0.1729	1.0209	0.4173	0.104*
H21B	0.2918	0.9357	0.4634	0.104*
H21C	0.3085	1.0505	0.3967	0.104*
C22	0.2845 (4)	0.9979 (4)	0.6854 (4)	0.0512 (10)
H22A	0.2848	1.0450	0.7582	0.061*
H22B	0.1969	0.9652	0.6509	0.061*
C23	0.3830 (4)	0.9025 (4)	0.7313 (4)	0.0506 (10)
H23A	0.4695	0.9357	0.7710	0.061*
H23B	0.3875	0.8592	0.6574	0.061*
C24	0.3533 (4)	0.8201 (4)	0.8264 (3)	0.0431 (9)
H24	0.2646	0.7883	0.7882	0.052*
C25	0.4510 (4)	0.7234 (4)	0.8664 (4)	0.0512 (10)
H25	0.4499	0.6826	0.7881	0.061*
C26	0.4119 (5)	0.6376 (5)	0.9527 (5)	0.0665 (12)
H26A	0.4240	0.6712	1.0353	0.100*
H26B	0.4663	0.5707	0.9621	0.100*
H26C	0.3208	0.6167	0.9150	0.100*
C27	0.5931 (4)	0.7633 (5)	0.9299 (5)	0.0678 (14)
H27A	0.6240	0.8032	0.8683	0.102*
H27B	0.6486	0.6984	0.9615	0.102*
H27C	0.5958	0.8135	0.9998	0.102*
C28	0.2567 (4)	0.8735 (4)	0.9903 (4)	0.0469 (9)
C29	0.2819 (5)	0.9406 (5)	1.1110 (4)	0.0606 (11)
H29A	0.2001	0.9525	1.1289	0.091*
H29B	0.3197	1.0131	1.1011	0.091*
H29C	0.3421	0.8996	1.1805	0.091*
O1W	0.0684 (19)	0.5921 (16)	0.7944 (15)	0.298 (8)
H1W	0.095 (5)	0.658 (5)	0.846 (5)	0.126 (14)*
H2W	0.082 (5)	0.520 (5)	0.850 (5)	0.125 (14)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.083 (2)	0.059 (2)	0.0609 (18)	0.0183 (19)	0.0247 (16)	0.0202 (17)

O2	0.0548 (16)	0.0564 (19)	0.0486 (14)	−0.0057 (14)	0.0061 (12)	0.0047 (14)
O3	0.0443 (13)	0.0523 (16)	0.0420 (12)	−0.0032 (13)	0.0172 (10)	0.0013 (12)
O4	0.0548 (17)	0.075 (2)	0.081 (2)	−0.0157 (17)	0.0318 (16)	−0.0098 (19)
C1	0.057 (2)	0.052 (2)	0.0351 (17)	0.0089 (19)	0.0152 (16)	0.0070 (17)
C2	0.056 (2)	0.055 (3)	0.0396 (17)	0.0035 (19)	0.0134 (16)	0.0063 (19)
C3	0.0464 (19)	0.048 (2)	0.051 (2)	0.0047 (18)	0.0191 (16)	0.0085 (19)
C4	0.053 (2)	0.046 (2)	0.050 (2)	0.0008 (19)	0.0175 (16)	−0.0020 (18)
C5	0.0432 (18)	0.045 (2)	0.0396 (17)	−0.0037 (16)	0.0096 (14)	−0.0005 (16)
C6	0.068 (3)	0.050 (3)	0.0430 (19)	−0.001 (2)	0.0083 (18)	−0.0088 (19)
C7	0.067 (3)	0.049 (3)	0.0355 (18)	−0.003 (2)	0.0028 (17)	−0.0022 (18)
C8	0.0413 (18)	0.048 (2)	0.0377 (16)	−0.0021 (17)	0.0066 (14)	0.0011 (17)
C9	0.0404 (17)	0.045 (2)	0.0319 (15)	0.0024 (15)	0.0111 (13)	0.0018 (15)
C10	0.0414 (17)	0.046 (2)	0.0375 (16)	0.0006 (16)	0.0146 (14)	0.0039 (16)
C11	0.073 (3)	0.052 (3)	0.0299 (16)	0.005 (2)	0.0139 (16)	0.0009 (18)
C12	0.071 (3)	0.049 (3)	0.0322 (17)	0.005 (2)	0.0112 (17)	0.0005 (16)
C13	0.0447 (18)	0.047 (2)	0.0314 (16)	0.0037 (17)	0.0123 (14)	0.0033 (15)
C14	0.0454 (18)	0.049 (2)	0.0318 (16)	−0.0012 (17)	0.0098 (14)	0.0019 (16)
C15	0.074 (3)	0.056 (3)	0.0367 (19)	0.000 (2)	0.0055 (18)	0.0004 (19)
C16	0.068 (3)	0.061 (3)	0.0293 (17)	0.008 (2)	0.0111 (16)	0.0047 (17)
C17	0.0399 (18)	0.055 (2)	0.0373 (16)	0.0033 (17)	0.0135 (14)	0.0069 (17)
C18	0.057 (2)	0.066 (3)	0.070 (3)	0.011 (2)	0.034 (2)	0.019 (2)
C19	0.052 (2)	0.062 (3)	0.075 (3)	0.002 (2)	0.033 (2)	0.021 (2)
C20	0.0468 (19)	0.055 (3)	0.0399 (18)	0.0019 (17)	0.0170 (15)	0.0068 (17)
C21	0.102 (4)	0.057 (3)	0.047 (2)	0.009 (3)	0.019 (2)	0.004 (2)
C22	0.051 (2)	0.057 (3)	0.050 (2)	0.007 (2)	0.0226 (17)	0.013 (2)
C23	0.0486 (19)	0.061 (3)	0.0473 (19)	0.0073 (19)	0.0224 (16)	0.0138 (19)
C24	0.0443 (18)	0.049 (2)	0.0371 (17)	−0.0001 (16)	0.0143 (14)	0.0009 (16)
C25	0.057 (2)	0.054 (3)	0.0428 (18)	0.007 (2)	0.0154 (16)	0.0069 (18)
C26	0.078 (3)	0.054 (3)	0.069 (3)	0.011 (2)	0.025 (2)	0.016 (2)
C27	0.053 (2)	0.082 (4)	0.066 (3)	0.014 (2)	0.015 (2)	0.024 (3)
C28	0.0479 (19)	0.051 (2)	0.0458 (18)	0.0047 (19)	0.0208 (15)	0.0089 (18)
C29	0.076 (3)	0.061 (3)	0.051 (2)	0.006 (2)	0.029 (2)	0.004 (2)
O1W	0.349 (18)	0.22 (2)	0.308 (19)	0.027 (17)	0.074 (15)	−0.006 (18)

Geometric parameters (Å, º)

O1—C3	1.223 (5)	C16—C17	1.549 (5)
O2—C1	1.431 (5)	C16—H16A	0.9700
O2—C2	1.451 (5)	C16—H16B	0.9700
O3—C28	1.339 (4)	C17—C20	1.530 (6)
O3—C24	1.462 (4)	C17—H17	0.9800
O4—C28	1.194 (5)	C18—H18A	0.9600
C1—C2	1.456 (6)	C18—H18B	0.9600
C1—C10	1.526 (5)	C18—H18C	0.9600
C1—H1	0.9800	C19—H19A	0.9600
C2—C3	1.475 (6)	C19—H19B	0.9600
C2—H2	0.9800	C19—H19C	0.9600
C3—C4	1.465 (6)	C20—C21	1.524 (6)

C4—C5	1.339 (6)	C20—C22	1.529 (5)
C4—H4	0.9300	C20—H20	0.9800
C5—C6	1.449 (5)	C21—H21A	0.9600
C5—C10	1.515 (6)	C21—H21B	0.9600
C6—C7	1.342 (6)	C21—H21C	0.9600
C6—H6	0.9300	C22—C23	1.509 (6)
C7—C8	1.481 (6)	C22—H22A	0.9700
C7—H7	0.9300	C22—H22B	0.9700
C8—C14	1.527 (6)	C23—C24	1.525 (5)
C8—C9	1.543 (5)	C23—H23A	0.9700
C8—H8	0.9800	C23—H23B	0.9700
C9—C11	1.533 (6)	C24—C25	1.509 (6)
C9—C10	1.548 (5)	C24—H24	0.9800
C9—H9	0.9800	C25—C27	1.529 (6)
C10—C19	1.535 (5)	C25—C26	1.526 (6)
C11—C12	1.515 (6)	C25—H25	0.9800
C11—H11A	0.9700	C26—H26A	0.9600
C11—H11B	0.9700	C26—H26B	0.9600
C12—C13	1.541 (5)	C26—H26C	0.9600
C12—H12A	0.9700	C27—H27A	0.9600
C12—H12B	0.9700	C27—H27B	0.9600
C13—C18	1.527 (5)	C27—H27C	0.9600
C13—C14	1.535 (6)	C28—C29	1.492 (6)
C13—C17	1.554 (5)	C29—H29A	0.9600
C14—C15	1.522 (5)	C29—H29B	0.9600
C14—H14	0.9800	C29—H29C	0.9600
C15—C16	1.522 (7)	O1W—H1W	0.94 (5)
C15—H15A	0.9700	O1W—H2W	1.03 (5)
C15—H15B	0.9700		

C1—O2—C2	60.7 (3)	C15—C16—H16B	110.2
C28—O3—C24	119.0 (3)	C17—C16—H16B	110.2
O2—C1—C2	60.3 (3)	H16A—C16—H16B	108.5
O2—C1—C10	117.9 (3)	C20—C17—C16	112.2 (3)
C2—C1—C10	122.0 (4)	C20—C17—C13	120.7 (3)
O2—C1—H1	115.2	C16—C17—C13	102.9 (3)
C2—C1—H1	115.2	C20—C17—H17	106.8
C10—C1—H1	115.2	C16—C17—H17	106.8
O2—C2—C1	59.0 (3)	C13—C17—H17	106.8
O2—C2—C3	113.3 (3)	C13—C18—H18A	109.5
C1—C2—C3	118.9 (3)	C13—C18—H18B	109.5
O2—C2—H2	117.4	H18A—C18—H18B	109.5
C1—C2—H2	117.4	C13—C18—H18C	109.5
C3—C2—H2	117.4	H18A—C18—H18C	109.5
O1—C3—C4	123.3 (4)	H18B—C18—H18C	109.5
O1—C3—C2	120.8 (4)	C10—C19—H19A	109.5
C4—C3—C2	115.9 (4)	C10—C19—H19B	109.5
C5—C4—C3	123.7 (4)	H19A—C19—H19B	109.5

C5—C4—H4	118.1	C10—C19—H19C	109.5
C3—C4—H4	118.1	H19A—C19—H19C	109.5
C4—C5—C6	119.7 (4)	H19B—C19—H19C	109.5
C4—C5—C10	122.9 (3)	C21—C20—C17	113.6 (3)
C6—C5—C10	117.3 (4)	C21—C20—C22	110.4 (4)
C7—C6—C5	123.3 (4)	C17—C20—C22	111.1 (3)
C7—C6—H6	118.4	C21—C20—H20	107.1
C5—C6—H6	118.4	C17—C20—H20	107.1
C6—C7—C8	122.3 (3)	C22—C20—H20	107.1
C6—C7—H7	118.8	C20—C21—H21A	109.5
C8—C7—H7	118.8	C20—C21—H21B	109.5
C7—C8—C14	114.4 (3)	H21A—C21—H21B	109.5
C7—C8—C9	110.9 (3)	C20—C21—H21C	109.5
C14—C8—C9	108.4 (3)	H21A—C21—H21C	109.5
C7—C8—H8	107.6	H21B—C21—H21C	109.5
C14—C8—H8	107.6	C23—C22—C20	113.9 (3)
C9—C8—H8	107.6	C23—C22—H22A	108.8
C11—C9—C8	111.6 (3)	C20—C22—H22A	108.8
C11—C9—C10	114.8 (3)	C23—C22—H22B	108.8
C8—C9—C10	110.8 (3)	C20—C22—H22B	108.8
C11—C9—H9	106.3	H22A—C22—H22B	107.7
C8—C9—H9	106.3	C22—C23—C24	115.3 (3)
C10—C9—H9	106.3	C22—C23—H23A	108.4
C5—C10—C1	110.1 (3)	C24—C23—H23A	108.4
C5—C10—C19	107.8 (4)	C22—C23—H23B	108.4
C1—C10—C19	107.3 (3)	C24—C23—H23B	108.4
C5—C10—C9	108.8 (3)	H23A—C23—H23B	107.5
C1—C10—C9	110.4 (3)	O3—C24—C25	108.9 (3)
C19—C10—C9	112.4 (3)	O3—C24—C23	107.2 (3)
C12—C11—C9	113.4 (3)	C25—C24—C23	113.8 (3)
C12—C11—H11A	108.9	O3—C24—H24	109.0
C9—C11—H11A	108.9	C25—C24—H24	109.0
C12—C11—H11B	108.9	C23—C24—H24	109.0
C9—C11—H11B	108.9	C24—C25—C27	113.5 (4)
H11A—C11—H11B	107.7	C24—C25—C26	112.3 (4)
C11—C12—C13	112.9 (4)	C27—C25—C26	109.9 (4)
C11—C12—H12A	109.0	C24—C25—H25	106.9
C13—C12—H12A	109.0	C27—C25—H25	106.9
C11—C12—H12B	109.0	C26—C25—H25	106.9
C13—C12—H12B	109.0	C25—C26—H26A	109.5
H12A—C12—H12B	107.8	C25—C26—H26B	109.5
C18—C13—C14	112.7 (4)	H26A—C26—H26B	109.5
C18—C13—C12	110.3 (3)	C25—C26—H26C	109.5
C14—C13—C12	106.6 (3)	H26A—C26—H26C	109.5
C18—C13—C17	110.0 (3)	H26B—C26—H26C	109.5
C14—C13—C17	100.1 (3)	C25—C27—H27A	109.5
C12—C13—C17	116.9 (3)	C25—C27—H27B	109.5
C15—C14—C8	119.2 (3)	H27A—C27—H27B	109.5

C15—C14—C13	104.3 (3)	C25—C27—H27C	109.5
C8—C14—C13	114.0 (3)	H27A—C27—H27C	109.5
C15—C14—H14	106.1	H27B—C27—H27C	109.5
C8—C14—H14	106.1	O4—C28—O3	124.6 (4)
C13—C14—H14	106.1	O4—C28—C29	124.3 (4)
C16—C15—C14	104.0 (3)	O3—C28—C29	111.0 (4)
C16—C15—H15A	111.0	C28—C29—H29A	109.5
C14—C15—H15A	111.0	C28—C29—H29B	109.5
C16—C15—H15B	111.0	H29A—C29—H29B	109.5
C14—C15—H15B	111.0	C28—C29—H29C	109.5
H15A—C15—H15B	109.0	H29A—C29—H29C	109.5
C15—C16—C17	107.6 (3)	H29B—C29—H29C	109.5
C15—C16—H16A	110.2	H1W—O1W—H2W	111 (6)
C17—C16—H16A	110.2		

C2—O2—C1—C10	112.9 (4)	C9—C11—C12—C13	−53.3 (5)
C1—O2—C2—C3	−110.8 (4)	C11—C12—C13—C18	−67.5 (5)
C10—C1—C2—O2	−106.2 (4)	C11—C12—C13—C14	55.1 (4)
O2—C1—C2—C3	101.3 (4)	C11—C12—C13—C17	165.9 (3)
C10—C1—C2—C3	−4.9 (6)	C7—C8—C14—C15	−51.6 (5)
O2—C2—C3—O1	−125.7 (4)	C9—C8—C14—C15	−175.9 (3)
C1—C2—C3—O1	168.1 (4)	C7—C8—C14—C13	−175.6 (3)
O2—C2—C3—C4	52.0 (5)	C9—C8—C14—C13	60.0 (4)
C1—C2—C3—C4	−14.3 (6)	C18—C13—C14—C15	−70.8 (4)
O1—C3—C4—C5	−168.8 (4)	C12—C13—C14—C15	168.1 (3)
C2—C3—C4—C5	13.6 (6)	C17—C13—C14—C15	45.9 (4)
C3—C4—C5—C6	−174.0 (4)	C18—C13—C14—C8	60.9 (4)
C3—C4—C5—C10	7.6 (6)	C12—C13—C14—C8	−60.2 (4)
C4—C5—C6—C7	174.4 (4)	C17—C13—C14—C8	177.6 (3)
C10—C5—C6—C7	−7.2 (6)	C8—C14—C15—C16	−162.1 (4)
C5—C6—C7—C8	0.2 (7)	C13—C14—C15—C16	−33.5 (4)
C6—C7—C8—C14	−145.8 (4)	C14—C15—C16—C17	7.6 (5)
C6—C7—C8—C9	−22.8 (6)	C15—C16—C17—C20	151.7 (4)
C7—C8—C9—C11	−179.3 (4)	C15—C16—C17—C13	20.5 (5)
C14—C8—C9—C11	−52.9 (4)	C18—C13—C17—C20	−47.0 (5)
C7—C8—C9—C10	51.4 (4)	C14—C13—C17—C20	−165.7 (3)
C14—C8—C9—C10	177.8 (3)	C12—C13—C17—C20	79.8 (4)
C4—C5—C10—C1	−25.0 (5)	C18—C13—C17—C16	78.9 (4)
C6—C5—C10—C1	156.6 (4)	C14—C13—C17—C16	−39.8 (4)
C4—C5—C10—C19	91.7 (4)	C12—C13—C17—C16	−154.3 (3)
C6—C5—C10—C19	−86.7 (4)	C16—C17—C20—C21	−174.5 (4)
C4—C5—C10—C9	−146.1 (4)	C13—C17—C20—C21	−53.1 (5)
C6—C5—C10—C9	35.4 (4)	C16—C17—C20—C22	60.3 (4)
O2—C1—C10—C5	−47.5 (5)	C13—C17—C20—C22	−178.3 (3)
C2—C1—C10—C5	23.3 (5)	C21—C20—C22—C23	77.8 (5)
O2—C1—C10—C19	−164.6 (4)	C17—C20—C22—C23	−155.3 (4)
C2—C1—C10—C19	−93.8 (4)	C20—C22—C23—C24	−175.9 (4)
O2—C1—C10—C9	72.7 (4)	C28—O3—C24—C25	−103.7 (4)

C2—C1—C10—C9	143.5 (4)	C28—O3—C24—C23	132.7 (3)
C11—C9—C10—C5	175.0 (3)	C22—C23—C24—O3	−61.7 (4)
C8—C9—C10—C5	−57.4 (4)	C22—C23—C24—C25	177.9 (4)
C11—C9—C10—C1	54.1 (4)	O3—C24—C25—C27	−60.1 (4)
C8—C9—C10—C1	−178.3 (3)	C23—C24—C25—C27	59.4 (5)
C11—C9—C10—C19	−65.7 (4)	O3—C24—C25—C26	65.2 (5)
C8—C9—C10—C19	61.9 (4)	C23—C24—C25—C26	−175.3 (4)
C8—C9—C11—C12	51.4 (5)	C24—O3—C28—O4	−3.0 (6)
C10—C9—C11—C12	178.6 (4)	C24—O3—C28—C29	175.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O4	0.95 (6)	2.15 (6)	3.085 (18)	174 (5)
O1*W*—H2*W*···O1^{i}	1.03 (6)	1.78 (6)	2.799 (18)	170 (5)
C1—H1···O1^{ii}	0.98	2.46	3.430 (6)	169

Symmetry codes: (i) −*x*, *y*−3/2, −*z*+1; (ii) −*x*, *y*−1/2, −*z*.