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# 3-*epi*-Dammarenediol II 1.075 hydrate: a dammarane triterpene from the bark of *Aglaia eximia*

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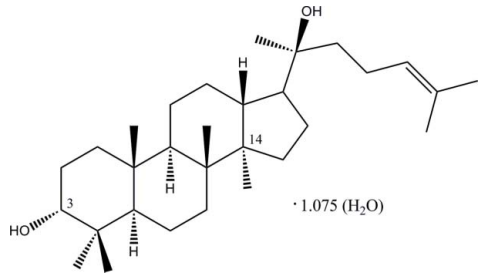
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.058; $wR$ factor = 0.162; data-to-parameter ratio = 13.7.

The title dammarane tritepene, 3$\alpha$,20(S)-dihydroxydammar-24-ene, which crystallized out in a hydrated form, $C_{30}H_{52}O_2.1.075H_2O$, was isolated from the *Aglaia eximia* bark. The three cyclohexane rings adopt chair conformations. The cyclopentane has an envelope conformation with the quaternary C at position 14 as the flap atom with the maximum deviation of 0.288 (2) Å. The methylheptene side chain is disordered over two positions with 0.505 (1):0.495 (1) site occupancies and is axially attached with an (+)-*syn-clinal* conformation. The hydroxyl group at position 3 of dammarane is in a different conformation to the corresponding hydroxyl in Dammarenediol II. In the crystal, the dammarane and water molecules are linked by $O_{Dammarane}—H\cdots O_{water}$ and $O_{water}—H\cdots O_{Dammarane}$ hydrogen bonds into a three-dimensional network.

## Related literature

For ring conformations, see: Cremer & Pople (1975). For bond-length data, see: Allen *et al.* (1987). For background to *Aglaia* plants, triterpenoids and their biological activity, see: Asakawa *et al.* (1977); Chairgulprasert *et al.* (2006); Greger *et al.* (2001); Grosvenor *et al.* (1995); Lima *et al.* (2004); Qiu *et al.* (2001); Roux *et al.* (1998); Yodsaoue *et al.* (2012); Zhang *et al.* (2010). For related structures, see: Qiu *et al.* (2001). For the stability of the temperature controller used in the data collection, see Cosier & Glazer (1986).




## Experimental

### Crystal data

$C_{30}H_{52}O_2·1.075H_2O$
$M_r$ = 463.99
Tetragonal, $P4_2$
$a$ = 19.9481 (13) Å
$c$ = 7.3410 (7) Å
$V$ = 2921.2 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 100 K
0.39 × 0.11 × 0.10 mm

### Data collection

Bruker APEX Duo CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.975, $T_{max}$ = 0.994
24864 measured reflections
4543 independent reflections
3887 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.064

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.162
$S$ = 1.07
4543 reflections
332 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.72 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.48 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H1*O2*···O1*W* | 0.84 | 2.02 | 2.816 (3) | 157 |
| O1*W*—H1*W*1···O1$^{i}$ | 0.84 | 1.94 | 2.783 (3) | 175 |
| O2*W*—H1*W*2···O2$^{ii}$ | 0.83 | 1.89 | 2.718 (3) | 177 |

Symmetry codes: (i) $y, -x+1, z+\frac{1}{2}$; (ii) $x, y, z+1$.

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2209).

‡ Thomson Reuters ResearcherID: A-3561-2009.
§ Thomson Reuters ResearcherID: A-5085-2009.

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# supplementary materials

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## 3-*epi*-Dammarenediol II 1.075 hydrate: a dammarane triterpene from the bark of *Aglaia eximia*

**Hoong-Kun Fun, Suchada Chantrapromma, Asep Supriadin, Desi Harneti and Unang Supratman**

### Comment

*Aglaia* genus plants belonging to the Mahogany family have been known as a good source of organic acids, sesquiterpenes, diterpenes and triterpenes (Chairgulprasert *et al.*, 2006; Qiu *et al.*, 2001; Roux *et al.*, 1998; Yodsaoue *et al.*, 2012). Many of the various terpenenoids from this genus possess interesting biological properties such as anti-inflammatory (Yodsaoue *et al.*, 2012), cytotoxic (Zhang *et al.*, 2010) and insecticidal (Greger *et al.*, 2001) activities. The title compound (I), 3-*epi*-Dammarenediol II or 3*α*,20(S)-dihydroxydammar-24-ene, was previously isolated from *Trattinnickia burserifolia* (Lima *et al.*, 2004). However it is now isolated for the first time from *Aglaia eximia*, a plant which was used as a traditional medicine for the treatment of malaria in Indonesia (Grosvenor *et al.*, 1995). Herein the crystal structure of (I) is reported.

Compound (I) has a dammarane nucleus and crystallized in a hydrated form, $C_{30}H_{52}O_2.1.075(H_2O)$ (Fig. 1). Two of the water molecules, O1W and O2W, have half occupancies and lie on two-fold axis, the other H of each water molecule was generated by a symmetry operation, -x, -y, z, whereas the third water molecule, O3W, has 0.075 occupancy. The molecule of dammarane has four fused rings and all rings are in *trans*-fused conformation. The three cyclohexane rings are in standard chair conformations. The cyclopentane (C13–C17) adopts an envelope conformation with the puckered C14 atom having the maximum deviation of 0.288 (2) Å, Q = 0.457 (3) Å and $\theta$ = 220.1 (3)° (Cremer & Pople, 1975). The hydroxyl group at atom C3 is axially attached which is different from the corresponding hydroxyl group in Dammarenediol II (Asakawa *et al.*, 1977). The methylheptene side chain is disordered over two positions; the major component and the minor component *A* (Fig. 1), with the refined site-occupancy ratio of 0.505 (1)/0.495 (1) and is axially attached at atom C20 with the torsion angle of C17–C20–C22–C23 = 58.83 (3)°, indicating an (+)-syn-clinal conformation with respect to the cyclopentane ring (Fig. 1). The bond distances in (I) are within normal ranges (Allen *et al.*, 1987) and comparable to a related structure (Qiu *et al.*, 2001).

The crystal packing of (I) is consolidated by intermolecular $O_{Dammarane}$—H···$O_{water}$ and $O_{water}$—H···$O_{Dammarane}$ hydrogen bonds (Table 1). The molecules of 3-*epi*-Dammarenediol II and water molecules are linked by O—H···O hydrogen bonds into a three dimensional network (Fig. 2).

### Experimental

The dried and milled bark of *A. eximia* (3 kg) which was collected from Bogor Botanical Garden, West Java, Indonesia, was extracted successively by n-hexane, ethyl acetate and methanol at room temperature. The ethyl acetate extract (300 g) was subjected to vacuum chromatography on silica gel G 60 by using a step gradient of n-hexane-ethyl acetate methanol. The fraction eluted by n-hexane/ethyl acetate (3:2) was further separated by column chromatography on silica gel (chloroform: methanol; 9.5:0.5 v/v) to give a colorless solid (63 mg) of the title compound. Colorless needle-shaped single crystals of the title compound suitable for X-ray structure determination were recrystallized from ethyl acetate at

room temperature after several days.

### Refinement

One of the water molecules, O3W, was refined isotropically. H atoms were positioned geometrically and allowed to ride on their parent atoms, with d(O—H) = 0.83-0.84 Å, d(C—H) = 1.00 Å for cyclic CH, 0.95 for CH, 0.99 for $CH_2$ and 0.98 Å for $CH_3$ atoms. The $U_{iso}$ values were constrained to be $1.2U_{eq}$ of the carrier atom for all H atoms. A rotating group model was used for the methyl groups. A total of 3923 Friedel pairs were merged before final refinement. The methyl-heptene side chain is disordered over two sites with refined site occupancies of 0.505 (1) and 0.495 (1). The same $U_{ij}$ parameters were used for atom pairs C23/C24, C26/C27 and C26A/C27A. A number of reflections were omitted from the final refinement owing to poor agreement.

### Computing details

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

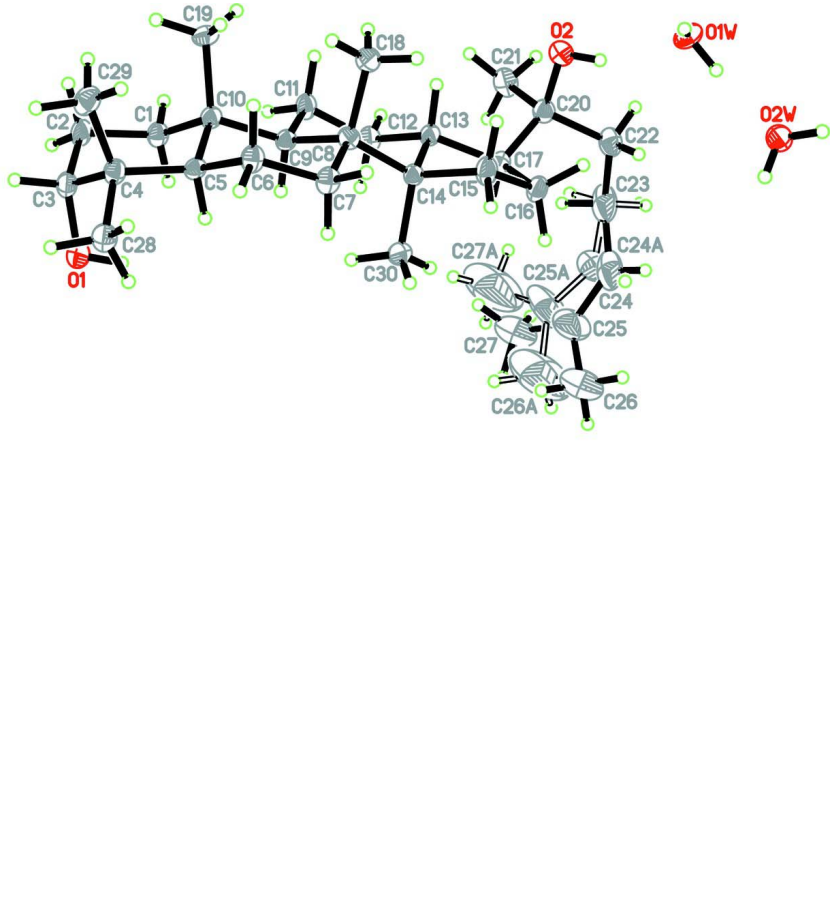


**Figure 1**

The molecular structure of the title compound, showing 60% probability displacement ellipsoids and the atom-numbering scheme. One H atom each of the O1W and O2W water molecules was generated by a symmetry operation -x, -y, z. Open bonds show the minor component.

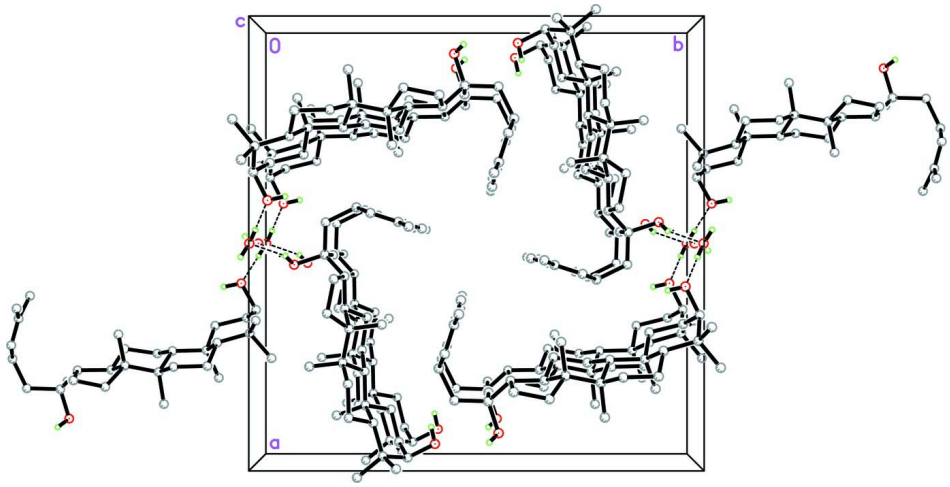


**Figure 2**

The crystal packing of the major component viewed along the *c* axis, only hydroxyl H and H atoms involving in hydrogen bonds are shown for clarity. O—H···O hydrogen bonds were drawn as dashed lines.

### 3*α*,20(*S*)-Dihydroxydammar-24-ene 1.075 hydrate

*Crystal data*

$C_{30}H_{52}O_2 \cdot 1.075H_2O$
$M_r = 463.99$
Tetragonal, $P4_2$
Hall symbol: P 4c
$a = 19.9481\ (13)$ Å
$c = 7.3410\ (7)$ Å
$V = 2921.2\ (5)$ Å$^3$
$Z = 4$
$F(000) = 1035$
$D_x = 1.055$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4543 reflections
$\theta = 2.0$–$30.0°$
$\mu = 0.07$ mm$^{-1}$
$T = 100$ K
Needle, colourless
0.39 × 0.11 × 0.10 mm

*Data collection*

Bruker APEX Duo CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.975$, $T_{max} = 0.994$
24864 measured reflections
4543 independent reflections
3887 reflections with $I > 2\sigma(I)$
$R_{int} = 0.064$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.0°$
$h = -28 \rightarrow 27$
$k = -22 \rightarrow 28$
$l = -10 \rightarrow 10$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.162$
$S = 1.07$
4543 reflections
332 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1014P)^2 + 0.4141P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.72$ e Å$^{-3}$
$\Delta\rho_{min} = -0.48$ e Å$^{-3}$
Absolute structure: nd

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O1 | 0.40685 (8) | 0.04934 (8) | 0.2210 (3) | 0.0194 (4) | |
| H1O1 | 0.3988 | 0.0883 | 0.2587 | 0.023* | |
| O2 | 0.09002 (8) | 0.45212 (8) | 0.2073 (3) | 0.0202 (4) | |
| H1O2 | 0.0731 | 0.4721 | 0.2969 | 0.024* | |
| C1 | 0.30479 (11) | 0.12044 (11) | 0.0082 (4) | 0.0158 (4) | |
| H1A | 0.2901 | 0.1373 | −0.1122 | 0.019* | |
| H1B | 0.3454 | 0.1457 | 0.0439 | 0.019* | |
| C2 | 0.32266 (12) | 0.04584 (12) | −0.0089 (3) | 0.0175 (5) | |
| H2A | 0.2832 | 0.0208 | −0.0543 | 0.021* | |
| H2B | 0.3593 | 0.0404 | −0.0987 | 0.021* | |
| C3 | 0.34456 (12) | 0.01670 (11) | 0.1731 (4) | 0.0160 (4) | |
| H3A | 0.3534 | −0.0323 | 0.1566 | 0.019* | |
| C4 | 0.29152 (12) | 0.02521 (11) | 0.3236 (4) | 0.0155 (4) | |
| C5 | 0.27016 (11) | 0.10018 (11) | 0.3325 (3) | 0.0133 (4) | |
| H5A | 0.3118 | 0.1245 | 0.3697 | 0.016* | |
| C6 | 0.21933 (12) | 0.11581 (11) | 0.4842 (4) | 0.0164 (4) | |
| H6A | 0.1741 | 0.1007 | 0.4466 | 0.020* | |
| H6B | 0.2319 | 0.0914 | 0.5965 | 0.020* | |
| C7 | 0.21811 (12) | 0.19144 (11) | 0.5223 (4) | 0.0164 (4) | |
| H7A | 0.2623 | 0.2051 | 0.5715 | 0.020* | |
| H7B | 0.1840 | 0.2007 | 0.6170 | 0.020* | |
| C8 | 0.20235 (11) | 0.23448 (11) | 0.3524 (3) | 0.0135 (4) | |
| C9 | 0.24808 (11) | 0.21167 (10) | 0.1905 (3) | 0.0132 (4) | |
| H9A | 0.2946 | 0.2217 | 0.2330 | 0.016* | |
| C10 | 0.24882 (11) | 0.13407 (11) | 0.1492 (3) | 0.0137 (4) | |
| C11 | 0.23870 (12) | 0.25678 (11) | 0.0224 (4) | 0.0164 (4) | |
| H11A | 0.1925 | 0.2511 | −0.0247 | 0.020* | |
| H11B | 0.2702 | 0.2423 | −0.0742 | 0.020* | |
| C12 | 0.25087 (12) | 0.33151 (11) | 0.0648 (4) | 0.0167 (4) | |
| H12A | 0.2982 | 0.3385 | 0.1008 | 0.020* | |
| H12B | 0.2418 | 0.3589 | −0.0450 | 0.020* | |
| C13 | 0.20444 (11) | 0.35310 (11) | 0.2196 (3) | 0.0142 (4) | |
| H13A | 0.1576 | 0.3429 | 0.1800 | 0.017* | |
| C14 | 0.21829 (11) | 0.31048 (11) | 0.3922 (3) | 0.0136 (4) | |
| C15 | 0.17269 (12) | 0.34658 (12) | 0.5301 (4) | 0.0185 (5) | |

| | | | | | |
|---|---|---|---|---|---|
| H15A | 0.1845 | 0.3342 | 0.6567 | 0.022* | |
| H15B | 0.1249 | 0.3357 | 0.5083 | 0.022* | |
| C16 | 0.18674 (13) | 0.42168 (11) | 0.4941 (4) | 0.0183 (5) | |
| H16A | 0.2245 | 0.4376 | 0.5703 | 0.022* | |
| H16B | 0.1466 | 0.4490 | 0.5218 | 0.022* | |
| C17 | 0.20495 (12) | 0.42675 (11) | 0.2870 (4) | 0.0156 (4) | |
| H17A | 0.2518 | 0.4442 | 0.2769 | 0.019* | |
| C18 | 0.12704 (11) | 0.22514 (12) | 0.3090 (4) | 0.0183 (5) | |
| H18A | 0.1002 | 0.2512 | 0.3956 | 0.022* | |
| H18B | 0.1153 | 0.1776 | 0.3190 | 0.022* | |
| H18C | 0.1179 | 0.2408 | 0.1849 | 0.022* | |
| C19 | 0.18212 (12) | 0.10878 (12) | 0.0669 (4) | 0.0185 (5) | |
| H19A | 0.1909 | 0.0699 | −0.0113 | 0.022* | |
| H19B | 0.1616 | 0.1446 | −0.0054 | 0.022* | |
| H19C | 0.1516 | 0.0958 | 0.1654 | 0.022* | |
| C20 | 0.15827 (12) | 0.47476 (11) | 0.1821 (4) | 0.0166 (5) | |
| C21 | 0.17162 (13) | 0.47347 (13) | −0.0233 (4) | 0.0217 (5) | |
| H21A | 0.1578 | 0.4300 | −0.0731 | 0.026* | |
| H21B | 0.2196 | 0.4803 | −0.0458 | 0.026* | |
| H21C | 0.1460 | 0.5093 | −0.0824 | 0.026* | |
| C22 | 0.16225 (13) | 0.54729 (12) | 0.2552 (4) | 0.0219 (5) | |
| H22A | 0.1308 | 0.5752 | 0.1838 | 0.026* | |
| H22B | 0.1462 | 0.5472 | 0.3828 | 0.026* | |
| C23 | 0.23106 (15) | 0.58110 (14) | 0.2509 (7) | 0.0405 (9) | |
| H23A | 0.2262 | 0.6298 | 0.2290 | 0.049* | 0.505 (14) |
| H23B | 0.2590 | 0.5618 | 0.1526 | 0.049* | 0.505 (14) |
| H23C | 0.2503 | 0.5715 | 0.1294 | 0.049* | 0.495 (14) |
| H23D | 0.2227 | 0.6300 | 0.2552 | 0.049* | 0.495 (14) |
| C24 | 0.2660 (5) | 0.5675 (4) | 0.4513 (17) | 0.0405 (9) | 0.505 (14) |
| H24A | 0.2382 | 0.5748 | 0.5545 | 0.049* | 0.505 (14) |
| C25 | 0.3285 (5) | 0.5474 (5) | 0.486 (2) | 0.053 (3) | 0.505 (14) |
| C26 | 0.3527 (5) | 0.5366 (8) | 0.680 (2) | 0.083 (4) | 0.505 (14) |
| H26A | 0.3176 | 0.5503 | 0.7651 | 0.100* | 0.505 (14) |
| H26B | 0.3931 | 0.5634 | 0.7008 | 0.100* | 0.505 (14) |
| H26C | 0.3631 | 0.4890 | 0.6978 | 0.100* | 0.505 (14) |
| C27 | 0.3782 (5) | 0.5330 (7) | 0.339 (2) | 0.083 (4) | 0.505 (14) |
| H27A | 0.3692 | 0.4886 | 0.2867 | 0.100* | 0.505 (14) |
| H27B | 0.4237 | 0.5339 | 0.3894 | 0.100* | 0.505 (14) |
| H27C | 0.3744 | 0.5670 | 0.2429 | 0.100* | 0.505 (14) |
| C24A | 0.2789 (4) | 0.5695 (4) | 0.3779 (19) | 0.041 (3) | 0.495 (14) |
| H24B | 0.2655 | 0.5767 | 0.5006 | 0.050* | 0.495 (14) |
| C25A | 0.3409 (4) | 0.5498 (5) | 0.355 (3) | 0.073 (5) | 0.495 (14) |
| C26A | 0.3867 (5) | 0.5364 (7) | 0.512 (3) | 0.111 (6) | 0.495 (14) |
| H26D | 0.3610 | 0.5374 | 0.6262 | 0.133* | 0.495 (14) |
| H26E | 0.4217 | 0.5708 | 0.5165 | 0.133* | 0.495 (14) |
| H26F | 0.4074 | 0.4922 | 0.4977 | 0.133* | 0.495 (14) |
| C27A | 0.3696 (5) | 0.5328 (8) | 0.159 (3) | 0.111 (6) | 0.495 (14) |
| H27D | 0.4145 | 0.5521 | 0.1466 | 0.133* | 0.495 (14) |
| H27E | 0.3400 | 0.5517 | 0.0662 | 0.133* | 0.495 (14) |

| | | | | | |
|---|---|---|---|---|---|
| H27F | 0.3720 | 0.4840 | 0.1444 | 0.133* | 0.495 (14) |
| C28 | 0.32341 (12) | 0.00442 (12) | 0.5058 (4) | 0.0188 (5) | |
| H28A | 0.3460 | −0.0389 | 0.4914 | 0.023* | |
| H28B | 0.2884 | 0.0006 | 0.5990 | 0.023* | |
| H28C | 0.3561 | 0.0384 | 0.5433 | 0.023* | |
| C29 | 0.23313 (13) | −0.02388 (12) | 0.2882 (4) | 0.0212 (5) | |
| H29A | 0.2497 | −0.0701 | 0.2956 | 0.025* | |
| H29B | 0.2146 | −0.0157 | 0.1666 | 0.025* | |
| H29C | 0.1981 | −0.0170 | 0.3800 | 0.025* | |
| C30 | 0.29122 (12) | 0.32099 (12) | 0.4601 (4) | 0.0188 (5) | |
| H30A | 0.3048 | 0.3675 | 0.4376 | 0.023* | |
| H30B | 0.3213 | 0.2906 | 0.3945 | 0.023* | |
| H30C | 0.2936 | 0.3115 | 0.5909 | 0.023* | |
| O1W | 0.0000 | 0.5000 | 0.4726 (4) | 0.0189 (5) | |
| H1W1 | 0.0159 | 0.5297 | 0.5419 | 0.023* | |
| O2W | 0.0000 | 0.5000 | 0.9617 (4) | 0.0187 (5) | |
| H1W2 | 0.0278 | 0.4839 | 1.0342 | 0.022* | |
| O3W | 0.967 (2) | 0.016 (2) | 0.858 (7) | 0.069 (12)* | 0.07 |
| H1W3 | 0.9518 | 0.0223 | 0.9645 | 0.083* | 0.07 |
| H2W3 | 1.0084 | 0.0055 | 0.8469 | 0.083* | 0.07 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0211 (8) | 0.0185 (8) | 0.0188 (9) | 0.0018 (6) | −0.0003 (7) | −0.0031 (7) |
| O2 | 0.0176 (8) | 0.0214 (8) | 0.0215 (10) | 0.0016 (6) | −0.0002 (7) | −0.0016 (8) |
| C1 | 0.0201 (10) | 0.0153 (9) | 0.0119 (11) | 0.0026 (8) | 0.0011 (9) | 0.0000 (9) |
| C2 | 0.0245 (11) | 0.0172 (10) | 0.0108 (11) | 0.0040 (8) | 0.0002 (9) | −0.0032 (9) |
| C3 | 0.0209 (10) | 0.0133 (9) | 0.0139 (11) | 0.0034 (8) | −0.0001 (9) | −0.0017 (8) |
| C4 | 0.0196 (10) | 0.0134 (9) | 0.0136 (11) | 0.0006 (8) | 0.0001 (9) | −0.0001 (9) |
| C5 | 0.0160 (10) | 0.0150 (9) | 0.0089 (10) | 0.0004 (7) | −0.0002 (8) | −0.0010 (8) |
| C6 | 0.0202 (10) | 0.0152 (9) | 0.0139 (12) | 0.0008 (8) | 0.0035 (9) | 0.0002 (9) |
| C7 | 0.0219 (10) | 0.0170 (10) | 0.0103 (10) | 0.0013 (8) | 0.0028 (9) | 0.0012 (9) |
| C8 | 0.0143 (9) | 0.0163 (10) | 0.0098 (10) | 0.0021 (7) | 0.0006 (8) | 0.0009 (8) |
| C9 | 0.0155 (9) | 0.0135 (9) | 0.0106 (11) | 0.0013 (7) | −0.0004 (8) | −0.0006 (8) |
| C10 | 0.0157 (10) | 0.0145 (9) | 0.0109 (11) | 0.0007 (7) | 0.0000 (8) | −0.0009 (8) |
| C11 | 0.0220 (10) | 0.0162 (10) | 0.0109 (11) | 0.0038 (8) | 0.0015 (9) | 0.0000 (9) |
| C12 | 0.0210 (11) | 0.0164 (10) | 0.0127 (11) | 0.0025 (8) | 0.0024 (9) | 0.0022 (9) |
| C13 | 0.0168 (9) | 0.0146 (9) | 0.0112 (11) | 0.0022 (7) | −0.0013 (9) | −0.0018 (9) |
| C14 | 0.0166 (10) | 0.0139 (9) | 0.0101 (10) | 0.0032 (8) | −0.0011 (8) | −0.0015 (8) |
| C15 | 0.0244 (11) | 0.0179 (10) | 0.0133 (11) | 0.0044 (8) | 0.0029 (9) | −0.0017 (9) |
| C16 | 0.0264 (11) | 0.0153 (10) | 0.0131 (11) | 0.0045 (8) | −0.0025 (10) | −0.0025 (9) |
| C17 | 0.0181 (10) | 0.0135 (9) | 0.0151 (11) | 0.0013 (7) | −0.0005 (9) | −0.0029 (9) |
| C18 | 0.0156 (10) | 0.0197 (10) | 0.0197 (12) | −0.0001 (8) | 0.0013 (9) | −0.0025 (10) |
| C19 | 0.0183 (10) | 0.0205 (10) | 0.0167 (12) | −0.0009 (8) | −0.0063 (9) | −0.0021 (9) |
| C20 | 0.0185 (10) | 0.0153 (10) | 0.0161 (12) | 0.0019 (8) | 0.0001 (9) | 0.0010 (9) |
| C21 | 0.0266 (12) | 0.0228 (11) | 0.0157 (12) | 0.0060 (9) | 0.0029 (10) | 0.0043 (10) |
| C22 | 0.0238 (11) | 0.0149 (10) | 0.0272 (15) | 0.0023 (8) | 0.0022 (10) | 0.0007 (10) |
| C23 | 0.0309 (14) | 0.0176 (11) | 0.073 (3) | −0.0046 (9) | 0.0144 (16) | −0.0107 (14) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C24 | 0.0309 (14) | 0.0176 (11) | 0.073 (3) | −0.0046 (9) | 0.0144 (16) | −0.0107 (14) |
| C25 | 0.024 (4) | 0.047 (4) | 0.090 (9) | −0.003 (3) | −0.013 (5) | −0.006 (5) |
| C26 | 0.040 (4) | 0.102 (6) | 0.108 (9) | 0.019 (4) | −0.029 (4) | −0.032 (6) |
| C27 | 0.040 (4) | 0.102 (6) | 0.108 (9) | 0.019 (4) | −0.029 (4) | −0.032 (6) |
| C24A | 0.021 (3) | 0.022 (3) | 0.081 (8) | −0.006 (2) | −0.006 (4) | −0.007 (4) |
| C25A | 0.017 (4) | 0.036 (4) | 0.166 (17) | −0.003 (3) | 0.001 (6) | 0.007 (7) |
| C26A | 0.035 (4) | 0.091 (6) | 0.207 (18) | −0.008 (3) | −0.016 (6) | 0.018 (8) |
| C27A | 0.035 (4) | 0.091 (6) | 0.207 (18) | −0.008 (3) | −0.016 (6) | 0.018 (8) |
| C28 | 0.0238 (11) | 0.0178 (10) | 0.0149 (11) | 0.0024 (8) | 0.0000 (10) | 0.0012 (9) |
| C29 | 0.0261 (12) | 0.0150 (10) | 0.0224 (13) | −0.0030 (9) | −0.0012 (10) | −0.0004 (10) |
| C30 | 0.0198 (10) | 0.0167 (10) | 0.0197 (12) | 0.0005 (8) | −0.0056 (10) | −0.0016 (9) |
| O1W | 0.0233 (12) | 0.0190 (11) | 0.0145 (12) | −0.0064 (9) | 0.000 | 0.000 |
| O2W | 0.0190 (11) | 0.0212 (11) | 0.0158 (12) | 0.0021 (9) | 0.000 | 0.000 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C3 | 1.446 (3) | C18—H18C | 0.9800 |
| O1—H1O1 | 0.8400 | C19—H19A | 0.9800 |
| O2—C20 | 1.446 (3) | C19—H19B | 0.9800 |
| O2—H1O2 | 0.8400 | C19—H19C | 0.9800 |
| C1—C2 | 1.535 (3) | C20—C21 | 1.531 (4) |
| C1—C10 | 1.547 (3) | C20—C22 | 1.545 (3) |
| C1—H1A | 0.9900 | C21—H21A | 0.9800 |
| C1—H1B | 0.9900 | C21—H21B | 0.9800 |
| C2—C3 | 1.522 (3) | C21—H21C | 0.9800 |
| C2—H2A | 0.9900 | C22—C23 | 1.530 (4) |
| C2—H2B | 0.9900 | C22—H22A | 0.9900 |
| C3—C4 | 1.539 (3) | C22—H22B | 0.9900 |
| C3—H3A | 1.0000 | C23—C24A | 1.354 (11) |
| C4—C28 | 1.538 (4) | C23—C24 | 1.650 (13) |
| C4—C29 | 1.544 (3) | C23—H23A | 0.9900 |
| C4—C5 | 1.557 (3) | C23—H23B | 0.9900 |
| C5—C6 | 1.538 (3) | C23—H23C | 0.9900 |
| C5—C10 | 1.565 (3) | C23—H23D | 0.9899 |
| C5—H5A | 1.0000 | C24—C25 | 1.335 (13) |
| C6—C7 | 1.535 (3) | C24—H24A | 0.9500 |
| C6—H6A | 0.9900 | C25—C27 | 1.496 (19) |
| C6—H6B | 0.9900 | C25—C26 | 1.516 (19) |
| C7—C8 | 1.546 (3) | C26—H26A | 0.9800 |
| C7—H7A | 0.9900 | C26—H26B | 0.9800 |
| C7—H7B | 0.9900 | C26—H26C | 0.9800 |
| C8—C18 | 1.547 (3) | C27—H27A | 0.9800 |
| C8—C9 | 1.566 (3) | C27—H27B | 0.9800 |
| C8—C14 | 1.577 (3) | C27—H27C | 0.9800 |
| C9—C11 | 1.539 (3) | C24A—C25A | 1.309 (12) |
| C9—C10 | 1.577 (3) | C24A—H24B | 0.9500 |
| C9—H9A | 1.0000 | C25A—C26A | 1.50 (3) |
| C10—C19 | 1.546 (3) | C25A—C27A | 1.58 (3) |
| C11—C12 | 1.542 (3) | C26A—H26D | 0.9800 |
| C11—H11A | 0.9900 | C26A—H26E | 0.9800 |

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|---|---|---|---|
| C11—H11B | 0.9900 | C26A—H26F | 0.9800 |
| C12—C13 | 1.528 (3) | C27A—H27D | 0.9800 |
| C12—H12A | 0.9900 | C27A—H27E | 0.9800 |
| C12—H12B | 0.9900 | C27A—H27F | 0.9800 |
| C13—C17 | 1.550 (3) | C28—H28A | 0.9800 |
| C13—C14 | 1.551 (3) | C28—H28B | 0.9800 |
| C13—H13A | 1.0000 | C28—H28C | 0.9800 |
| C14—C15 | 1.540 (3) | C29—H29A | 0.9800 |
| C14—C30 | 1.552 (3) | C29—H29B | 0.9800 |
| C15—C16 | 1.547 (3) | C29—H29C | 0.9800 |
| C15—H15A | 0.9900 | C30—H30A | 0.9800 |
| C15—H15B | 0.9900 | C30—H30B | 0.9800 |
| C16—C17 | 1.566 (4) | C30—H30C | 0.9800 |
| C16—H16A | 0.9900 | O1W—H1W1 | 0.8422 |
| C16—H16B | 0.9900 | O2W—H1W2 | 0.8324 |
| C17—C20 | 1.542 (3) | O3W—O3W$^{i}$ | 1.45 (9) |
| C17—H17A | 1.0000 | O3W—H1W3 | 0.8496 |
| C18—H18A | 0.9800 | O3W—H2W3 | 0.8504 |
| C18—H18B | 0.9800 | | |

| | | | |
|---|---|---|---|
| C3—O1—H1O1 | 109.4 | C20—C17—C13 | 115.2 (2) |
| C20—O2—H1O2 | 109.3 | C20—C17—C16 | 112.63 (19) |
| C2—C1—C10 | 113.14 (19) | C13—C17—C16 | 104.30 (19) |
| C2—C1—H1A | 109.0 | C20—C17—H17A | 108.2 |
| C10—C1—H1A | 109.0 | C13—C17—H17A | 108.2 |
| C2—C1—H1B | 109.0 | C16—C17—H17A | 108.2 |
| C10—C1—H1B | 109.0 | C8—C18—H18A | 109.5 |
| H1A—C1—H1B | 107.8 | C8—C18—H18B | 109.5 |
| C3—C2—C1 | 111.4 (2) | H18A—C18—H18B | 109.5 |
| C3—C2—H2A | 109.3 | C8—C18—H18C | 109.5 |
| C1—C2—H2A | 109.3 | H18A—C18—H18C | 109.5 |
| C3—C2—H2B | 109.3 | H18B—C18—H18C | 109.5 |
| C1—C2—H2B | 109.3 | C10—C19—H19A | 109.5 |
| H2A—C2—H2B | 108.0 | C10—C19—H19B | 109.5 |
| O1—C3—C2 | 106.76 (19) | H19A—C19—H19B | 109.5 |
| O1—C3—C4 | 111.5 (2) | C10—C19—H19C | 109.5 |
| C2—C3—C4 | 113.01 (19) | H19A—C19—H19C | 109.5 |
| O1—C3—H3A | 108.5 | H19B—C19—H19C | 109.5 |
| C2—C3—H3A | 108.5 | O2—C20—C21 | 106.5 (2) |
| C4—C3—H3A | 108.5 | O2—C20—C17 | 108.10 (19) |
| C28—C4—C3 | 108.07 (19) | C21—C20—C17 | 112.1 (2) |
| C28—C4—C29 | 106.7 (2) | O2—C20—C22 | 107.25 (18) |
| C3—C4—C29 | 109.2 (2) | C21—C20—C22 | 110.4 (2) |
| C28—C4—C5 | 109.61 (19) | C17—C20—C22 | 112.2 (2) |
| C3—C4—C5 | 108.92 (18) | C20—C21—H21A | 109.5 |
| C29—C4—C5 | 114.21 (19) | C20—C21—H21B | 109.5 |
| C6—C5—C4 | 113.93 (19) | H21A—C21—H21B | 109.5 |
| C6—C5—C10 | 110.83 (18) | C20—C21—H21C | 109.5 |
| C4—C5—C10 | 116.96 (19) | H21A—C21—H21C | 109.5 |

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|---|---|---|---|
| C6—C5—H5A | 104.5 | H21B—C21—H21C | 109.5 |
| C4—C5—H5A | 104.5 | C23—C22—C20 | 116.9 (2) |
| C10—C5—H5A | 104.5 | C23—C22—H22A | 108.1 |
| C7—C6—C5 | 109.98 (19) | C20—C22—H22A | 108.1 |
| C7—C6—H6A | 109.7 | C23—C22—H22B | 108.1 |
| C5—C6—H6A | 109.7 | C20—C22—H22B | 108.1 |
| C7—C6—H6B | 109.7 | H22A—C22—H22B | 107.3 |
| C5—C6—H6B | 109.7 | C24A—C23—C22 | 122.9 (5) |
| H6A—C6—H6B | 108.2 | C22—C23—C24 | 106.7 (4) |
| C6—C7—C8 | 113.7 (2) | C24A—C23—H23A | 110.4 |
| C6—C7—H7A | 108.8 | C22—C23—H23A | 110.4 |
| C8—C7—H7A | 108.8 | C24—C23—H23A | 110.4 |
| C6—C7—H7B | 108.8 | C24A—C23—H23B | 92.3 |
| C8—C7—H7B | 108.8 | C22—C23—H23B | 110.4 |
| H7A—C7—H7B | 107.7 | C24—C23—H23B | 110.4 |
| C7—C8—C18 | 107.26 (19) | H23A—C23—H23B | 108.6 |
| C7—C8—C9 | 109.42 (17) | C24A—C23—H23C | 108.3 |
| C18—C8—C9 | 112.0 (2) | C22—C23—H23C | 106.4 |
| C7—C8—C14 | 110.1 (2) | C24—C23—H23C | 127.4 |
| C18—C8—C14 | 110.48 (18) | H23A—C23—H23C | 94.6 |
| C9—C8—C14 | 107.62 (18) | C24A—C23—H23D | 105.4 |
| C11—C9—C8 | 111.60 (17) | C22—C23—H23D | 106.4 |
| C11—C9—C10 | 114.9 (2) | C24—C23—H23D | 101.8 |
| C8—C9—C10 | 115.88 (18) | H23B—C23—H23D | 120.1 |
| C11—C9—H9A | 104.3 | H23C—C23—H23D | 106.5 |
| C8—C9—H9A | 104.3 | C25—C24—C23 | 127.9 (9) |
| C10—C9—H9A | 104.3 | C25—C24—H24A | 116.1 |
| C19—C10—C1 | 107.6 (2) | C23—C24—H24A | 116.1 |
| C19—C10—C5 | 115.41 (19) | C24—C25—C27 | 122.6 (12) |
| C1—C10—C5 | 107.65 (18) | C24—C25—C26 | 121.3 (12) |
| C19—C10—C9 | 112.78 (18) | C27—C25—C26 | 116.1 (8) |
| C1—C10—C9 | 107.94 (18) | C25A—C24A—C23 | 129.1 (13) |
| C5—C10—C9 | 105.14 (19) | C25A—C24A—H24B | 115.5 |
| C9—C11—C12 | 112.6 (2) | C23—C24A—H24B | 115.5 |
| C9—C11—H11A | 109.1 | C24A—C25A—C26A | 122.3 (17) |
| C12—C11—H11A | 109.1 | C24A—C25A—C27A | 121.4 (14) |
| C9—C11—H11B | 109.1 | C26A—C25A—C27A | 116.1 (11) |
| C12—C11—H11B | 109.1 | C25A—C26A—H26D | 109.5 |
| H11A—C11—H11B | 107.8 | C25A—C26A—H26E | 109.5 |
| C13—C12—C11 | 109.10 (19) | H26D—C26A—H26E | 109.5 |
| C13—C12—H12A | 109.9 | C25A—C26A—H26F | 109.5 |
| C11—C12—H12A | 109.9 | H26D—C26A—H26F | 109.5 |
| C13—C12—H12B | 109.9 | H26E—C26A—H26F | 109.5 |
| C11—C12—H12B | 109.9 | C25A—C27A—H27D | 109.5 |
| H12A—C12—H12B | 108.3 | C25A—C27A—H27E | 109.5 |
| C12—C13—C17 | 120.0 (2) | H27D—C27A—H27E | 109.5 |
| C12—C13—C14 | 110.19 (18) | C25A—C27A—H27F | 109.5 |
| C17—C13—C14 | 104.92 (19) | H27D—C27A—H27F | 109.5 |
| C12—C13—H13A | 107.0 | H27E—C27A—H27F | 109.5 |

| | | | |
|---|---|---|---|
| C17—C13—H13A | 107.0 | C4—C28—H28A | 109.5 |
| C14—C13—H13A | 107.0 | C4—C28—H28B | 109.5 |
| C15—C14—C13 | 100.11 (17) | H28A—C28—H28B | 109.5 |
| C15—C14—C30 | 106.2 (2) | C4—C28—H28C | 109.5 |
| C13—C14—C30 | 110.8 (2) | H28A—C28—H28C | 109.5 |
| C15—C14—C8 | 116.91 (19) | H28B—C28—H28C | 109.5 |
| C13—C14—C8 | 109.86 (19) | C4—C29—H29A | 109.5 |
| C30—C14—C8 | 112.24 (17) | C4—C29—H29B | 109.5 |
| C14—C15—C16 | 103.5 (2) | H29A—C29—H29B | 109.5 |
| C14—C15—H15A | 111.1 | C4—C29—H29C | 109.5 |
| C16—C15—H15A | 111.1 | H29A—C29—H29C | 109.5 |
| C14—C15—H15B | 111.1 | H29B—C29—H29C | 109.5 |
| C16—C15—H15B | 111.1 | C14—C30—H30A | 109.5 |
| H15A—C15—H15B | 109.0 | C14—C30—H30B | 109.5 |
| C15—C16—C17 | 105.70 (19) | H30A—C30—H30B | 109.5 |
| C15—C16—H16A | 110.6 | C14—C30—H30C | 109.5 |
| C17—C16—H16A | 110.6 | H30A—C30—H30C | 109.5 |
| C15—C16—H16B | 110.6 | H30B—C30—H30C | 109.5 |
| C17—C16—H16B | 110.6 | O3W$^{i}$—O3W—H1W3 | 113.1 |
| H16A—C16—H16B | 108.7 | H1W3—O3W—H2W3 | 118.4 |

| | | | |
|---|---|---|---|
| C10—C1—C2—C3 | −57.8 (3) | C11—C12—C13—C14 | 59.5 (2) |
| C1—C2—C3—O1 | −66.0 (2) | C12—C13—C14—C15 | 173.65 (18) |
| C1—C2—C3—C4 | 56.9 (3) | C17—C13—C14—C15 | 43.1 (2) |
| O1—C3—C4—C28 | −50.8 (2) | C12—C13—C14—C30 | 61.8 (2) |
| C2—C3—C4—C28 | −171.06 (19) | C17—C13—C14—C30 | −68.7 (2) |
| O1—C3—C4—C29 | −166.47 (19) | C12—C13—C14—C8 | −62.8 (2) |
| C2—C3—C4—C29 | 73.3 (2) | C17—C13—C14—C8 | 166.71 (17) |
| O1—C3—C4—C5 | 68.2 (2) | C7—C8—C14—C15 | −68.6 (2) |
| C2—C3—C4—C5 | −52.0 (3) | C18—C8—C14—C15 | 49.7 (3) |
| C28—C4—C5—C6 | −59.4 (3) | C9—C8—C14—C15 | 172.24 (19) |
| C3—C4—C5—C6 | −177.4 (2) | C7—C8—C14—C13 | 178.30 (18) |
| C29—C4—C5—C6 | 60.3 (3) | C18—C8—C14—C13 | −63.4 (2) |
| C28—C4—C5—C10 | 169.14 (19) | C9—C8—C14—C13 | 59.1 (2) |
| C3—C4—C5—C10 | 51.1 (3) | C7—C8—C14—C30 | 54.5 (3) |
| C29—C4—C5—C10 | −71.2 (3) | C18—C8—C14—C30 | 172.8 (2) |
| C4—C5—C6—C7 | 162.2 (2) | C9—C8—C14—C30 | −64.6 (3) |
| C10—C5—C6—C7 | −63.4 (2) | C13—C14—C15—C16 | −44.8 (2) |
| C5—C6—C7—C8 | 56.5 (3) | C30—C14—C15—C16 | 70.5 (2) |
| C6—C7—C8—C18 | 72.7 (2) | C8—C14—C15—C16 | −163.3 (2) |
| C6—C7—C8—C9 | −49.0 (3) | C14—C15—C16—C17 | 30.3 (2) |
| C6—C7—C8—C14 | −167.05 (18) | C12—C13—C17—C20 | 86.8 (3) |
| C7—C8—C9—C11 | −175.21 (18) | C14—C13—C17—C20 | −148.6 (2) |
| C18—C8—C9—C11 | 66.0 (2) | C12—C13—C17—C16 | −149.2 (2) |
| C14—C8—C9—C11 | −55.6 (2) | C14—C13—C17—C16 | −24.7 (2) |
| C7—C8—C9—C10 | 50.8 (3) | C15—C16—C17—C20 | 122.2 (2) |
| C18—C8—C9—C10 | −68.0 (2) | C15—C16—C17—C13 | −3.4 (2) |
| C14—C8—C9—C10 | 170.35 (18) | C13—C17—C20—O2 | 62.8 (3) |
| C2—C1—C10—C19 | −72.2 (2) | C16—C17—C20—O2 | −56.7 (2) |

| | | | |
|---|---|---|---|
| C2—C1—C10—C5 | 52.7 (2) | C13—C17—C20—C21 | −54.3 (3) |
| C2—C1—C10—C9 | 165.77 (19) | C16—C17—C20—C21 | −173.8 (2) |
| C6—C5—C10—C19 | −63.9 (3) | C13—C17—C20—C22 | −179.2 (2) |
| C4—C5—C10—C19 | 69.0 (3) | C16—C17—C20—C22 | 61.4 (3) |
| C6—C5—C10—C1 | 175.91 (17) | O2—C20—C22—C23 | 177.3 (3) |
| C4—C5—C10—C1 | −51.2 (2) | C21—C20—C22—C23 | −67.0 (3) |
| C6—C5—C10—C9 | 61.0 (2) | C17—C20—C22—C23 | 58.8 (3) |
| C4—C5—C10—C9 | −166.10 (18) | C20—C22—C23—C24A | −80.0 (6) |
| C11—C9—C10—C19 | −62.2 (3) | C20—C22—C23—C24 | −93.2 (4) |
| C8—C9—C10—C19 | 70.3 (3) | C24A—C23—C24—C25 | −12.1 (11) |
| C11—C9—C10—C1 | 56.5 (2) | C22—C23—C24—C25 | 134.1 (8) |
| C8—C9—C10—C1 | −170.92 (19) | C23—C24—C25—C27 | −0.7 (15) |
| C11—C9—C10—C5 | 171.24 (18) | C23—C24—C25—C26 | −179.4 (9) |
| C8—C9—C10—C5 | −56.2 (2) | C22—C23—C24A—C25A | 125.3 (8) |
| C8—C9—C11—C12 | 55.7 (3) | C24—C23—C24A—C25A | 165 (2) |
| C10—C9—C11—C12 | −169.78 (18) | C23—C24A—C25A—C26A | −177.2 (9) |
| C9—C11—C12—C13 | −56.3 (3) | C23—C24A—C25A—C27A | −2.7 (14) |
| C11—C12—C13—C17 | −178.5 (2) | | |

Symmetry code: (i) −*x*+2, −*y*, *z*.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H1*O2*···O1*W* | 0.84 | 2.02 | 2.816 (3) | 157 |
| O1*W*—H1*W*1···O1$^{ii}$ | 0.84 | 1.94 | 2.783 (3) | 175 |
| O2*W*—H1*W*2···O2$^{iii}$ | 0.83 | 1.89 | 2.718 (3) | 177 |

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