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# 3-(Biphenyl-1-yl)-1-(4-*tert*-butylphenyl)-3-hydroxyprop-2-en-1-one

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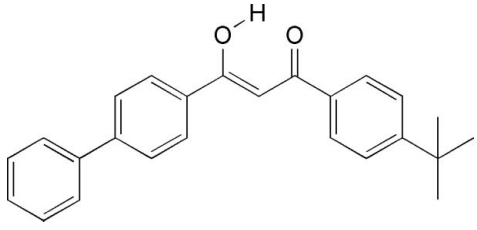
Key indicators: single-crystal X-ray study; $T$ = 292 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.056; $wR$ factor = 0.157; data-to-parameter ratio = 13.7.

In the title compound, $C_{25}H_{24}O_2$, the molecular structure exists in a *cis*-enol form which is stabilized by an intramolecular O—H···O hydrogen bond. This hydrogen bond is described as an approximately symmetrical hydrogen bond. The three methyl groups are disordered over two positions, with a site occupancy ratio of *ca* 4:1.

## Related literature

For related literature, see: Bertolasi *et al.* (1991); Gilli *et al.* (2004); Gorczynski *et al.* (2005); Hasegawa *et al.* (1997); Liang *et al.* (2003); Morris *et al.* (1996); Vila *et al.* (1991).



## Experimental

### *Crystal data*

$C_{25}H_{24}O_2$
$M_r$ = 356.44
Triclinic, $P\overline{1}$
$a$ = 6.5578 (6) Å
$b$ = 11.3548 (13) Å
$c$ = 14.1560 (13) Å
$\alpha$ = 99.040 (2)°
$\beta$ = 90.873 (2)°
$\gamma$ = 106.053 (2)°
$V$ = 998.49 (17) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 292 (2) K
0.20 × 0.10 × 0.10 mm

### *Data collection*

Bruker APEX CCD area-detector diffractometer
Absorption correction: none
6592 measured reflections
3845 independent reflections
2189 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.157
$S$ = 0.94
3845 reflections
281 parameters
48 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O2 | 1.28 (3) | 1.22 (3) | 2.453 (3) | 159 (3) |
| O1—H1···O2$^{i}$ | 1.28 (4) | 2.56 (3) | 3.183 (2) | 107.1 (17) |

Symmetry code: (i) $-x+2, -y+2, -z+2$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2173).

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# supplementary materials

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# 3-(Biphenyl-1-yl)-1-(4-*tert*-butylphenyl)-3-hydroxyprop-2-en-1-one

**C.-Y. Zheng, J. Zheng and D.-J. Wang**

## Comment

1,3-Diketones posses a broad spectrum of useful and sometimes unique chemical properties, which make them extremely attractive as intermediates (Hasegawa *et al.*, 1997; Morris *et al.*, 1996). They are also used widely in the chemistry of metallocomplexes (Gorczynski *et al.*, 2005; Liang *et al.*, 2003), and 1,3-diketones structure has received increasing attention for studying tautomerism (Vila *et al.*, 1991; Bertolasi *et al.*, 1991; Gilli *et al.*, 2004). The crystal structure of the title compound, (I), is in the enol form stabilized by an intramolecular hydrogen bond (Fig. 1 and Table 1). The distances of O1—H1 and O2—H1 are 1.28 (4) and 1.21 (3) Å, respectively. The central benzene ring (C14—C19) makes the dihedral angles of 4.22 (10) and 37.82 (11)° with benzene (C5—C10) and phenyl (C20—C25) rings, respectively.

## Experimental

1-(4-Phenylphenyl)ethanone (7.84 g, 0.04 mol), methyl 4-*tert*-butylbenzoate (7.68 g, 0.04 mol), $NaNH_2$ (1.95 g, 0.05 mol) and dry diethylether (60 ml) were mixed and stirred 6 h at room temperature under nitrogen. The mixture was then acidified with dilute hydrochloric acid and stirred until all solids dissolved. The ether layer was separated, washed with a saturated $NaHCO_3$ solution and dried over anhydrous $Na_2SO_4$. The solvent was removed by evaporation. The residual solid was recrystallized from an ethanol solution to give the title compound, (I) (yield 6.91 g, 48.5%; m.p. 396 K). Single crystals suitable for X-ray diffraction were grown by slow evaporation of a $CH_2Cl_2$—EtOH (2:1) solution at room temperature. $^1$H NMR ($CDCl_3$, 400 MHz): 1.38(s, 9H, $C(CH_3)_3$), 6.89(s, 1H, enol C—H), 7.40–7.50(m, 3H, Ar—H), 7.52(d, 2H, 8.4 Hz), 7.64–7.67(m, 2H), 7.72(d, 2H, 8.4 Hz, Ar—H), 7.95(d, 2H, 8.4 Hz), 8.06(d, 2H, 8.4 Hz), 16.95(br s, 1H, enol O—H). Analysis, calculated for $C_{25}H_{24}O_2$: C 84.24, H 6.79%; found: C 84.26, H 6.74%.

## Refinement

The methyl group was found to be disordered over two orientations. The occupancies of the disordered positions C1/C1', C2/C2' and C3/C3' were refined to 0.795 (5)/0.205 (5). Distance restraints (SADI) were applied for C—C distances of the disordered methyl groups and approximately isotropic restraints (ISOR) were used for C1'-C3'. The methyl H atoms were constrained to an ideal geometry with C—H = 0.96 Å, and with $U_{iso}$(H) = 1.5$U_{eq}$(C), but each group was allowed to rotate freely about its C—C bond. The H atom of the hydroxyl group was located in a difference Fourier map and its position was refined freely, with $U_{iso}$(H) = 1.5$U_{eq}$(O). Other H atoms were placed in geometrically idealized positions (C—H = 0.93 Å) and refined as riding, with $U_{iso}$(H) = 1.2$U_{eq}$(C).

## Figures

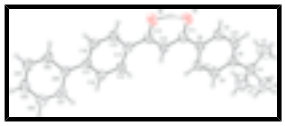

Fig. 1. The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. Only one component of the disordered methyl groups is shown. The dashed line indicates an intramolecular hydrogen bond.

## 3-(Biphenyl-1-yl)-1-(4-*tert*-butylphenyl)-3-hydroxyprop-2-en-1-one

### *Crystal data*

| | |
|---|---|
| $C_{25}H_{24}O_2$ | $Z = 2$ |
| $M_r = 356.44$ | $F_{000} = 380$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.186$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Melting point: 396 K |
| $a = 6.5578$ (6) Å | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $b = 11.3548$ (13) Å | Cell parameters from 1576 reflections |
| $c = 14.1560$ (13) Å | $\theta = 2.2$–$24.1^\circ$ |
| $\alpha = 99.040$ (2)° | $\mu = 0.07$ mm$^{-1}$ |
| $\beta = 90.873$ (2)° | $T = 292$ (2) K |
| $\gamma = 106.053$ (2)° | Block, colorless |
| $V = 998.49$ (17) Å$^3$ | 0.20 × 0.10 × 0.10 mm |

### *Data collection*

| | |
|---|---|
| Bruker APEX CCD area-detector diffractometer | 3845 independent reflections |
| Radiation source: fine-focus sealed tube | 2189 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.039$ |
| Detector resolution: 0 pixels mm$^{-1}$ | $\theta_{max} = 26.0^\circ$ |
| $T = 292(2)$ K | $\theta_{min} = 1.9^\circ$ |
| φ and ω scans | $h = -7 \rightarrow 8$ |
| Absorption correction: none | $k = -13 \rightarrow 13$ |
| 6592 measured reflections | $l = -13 \rightarrow 17$ |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.056$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.157$ | $w = 1/[\sigma^2(F_o^2) + (0.0781P)^2]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 0.94$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 3845 reflections | $\Delta\rho_{max} = 0.15$ e Å$^{-3}$ |

281 parameters
48 restraints
Primary atom site location: structure-invariant direct methods

$\Delta\rho_{min} = -0.20$ e Å$^{-3}$
Extinction correction: none

*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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1 | 0.1848 (7) | 1.1478 (4) | 0.4765 (3) | 0.132 (2) | 0.795 (5) |
| H1A | 0.0733 | 1.1238 | 0.5188 | 0.197* | 0.795 (5) |
| H1B | 0.2174 | 1.0750 | 0.4439 | 0.197* | 0.795 (5) |
| H1C | 0.1393 | 1.1902 | 0.4303 | 0.197* | 0.795 (5) |
| C2 | 0.3222 (8) | 1.3461 (4) | 0.5847 (3) | 0.126 (2) | 0.795 (5) |
| H2A | 0.2566 | 1.3792 | 0.5380 | 0.189* | 0.795 (5) |
| H2B | 0.4452 | 1.4088 | 0.6155 | 0.189* | 0.795 (5) |
| H2C | 0.2229 | 1.3206 | 0.6318 | 0.189* | 0.795 (5) |
| C3 | 0.5520 (7) | 1.2707 (6) | 0.4652 (3) | 0.150 (3) | 0.795 (5) |
| H3A | 0.4936 | 1.3017 | 0.4150 | 0.225* | 0.795 (5) |
| H3B | 0.5944 | 1.1987 | 0.4384 | 0.225* | 0.795 (5) |
| H3C | 0.6734 | 1.3338 | 0.4969 | 0.225* | 0.795 (5) |
| C1' | 0.1691 (13) | 1.2492 (14) | 0.5431 (11) | 0.101 (5) | 0.205 (5) |
| H1'1 | 0.1317 | 1.2811 | 0.4885 | 0.151* | 0.205 (5) |
| H1'2 | 0.1632 | 1.3055 | 0.6006 | 0.151* | 0.205 (5) |
| H1'3 | 0.0710 | 1.1694 | 0.5450 | 0.151* | 0.205 (5) |
| C2' | 0.547 (2) | 1.3667 (9) | 0.5480 (12) | 0.121 (6) | 0.205 (5) |
| H2'1 | 0.5053 | 1.4136 | 0.5043 | 0.181* | 0.205 (5) |
| H2'2 | 0.6867 | 1.3591 | 0.5346 | 0.181* | 0.205 (5) |
| H2'3 | 0.5496 | 1.4088 | 0.6126 | 0.181* | 0.205 (5) |
| C3' | 0.417 (3) | 1.1610 (13) | 0.4444 (7) | 0.116 (6) | 0.205 (5) |
| H3'1 | 0.3188 | 1.0796 | 0.4374 | 0.174* | 0.205 (5) |
| H3'2 | 0.5601 | 1.1540 | 0.4446 | 0.174* | 0.205 (5) |
| H3'3 | 0.3928 | 1.2006 | 0.3919 | 0.174* | 0.205 (5) |
| C4 | 0.3878 (4) | 1.2363 (2) | 0.53598 (17) | 0.0765 (7) | |
| C5 | 0.4578 (4) | 1.17304 (19) | 0.61368 (15) | 0.0641 (6) | |
| C6 | 0.3148 (4) | 1.0916 (2) | 0.65980 (17) | 0.0771 (7) | |
| H6 | 0.1705 | 1.0735 | 0.6430 | 0.092* | |
| C7 | 0.3788 (3) | 1.0358 (2) | 0.73024 (16) | 0.0714 (6) | |

| | | | | |
|---|---|---|---|---|
| H7 | 0.2772 | 0.9821 | 0.7604 | 0.086* |
| C8 | 0.5911 (3) | 1.05849 (18) | 0.75651 (14) | 0.0582 (5) |
| C9 | 0.7339 (4) | 1.1413 (2) | 0.71199 (17) | 0.0757 (7) |
| H9 | 0.8782 | 1.1599 | 0.7289 | 0.091* |
| C10 | 0.6680 (4) | 1.1978 (2) | 0.64268 (17) | 0.0780 (7) |
| H10 | 0.7694 | 1.2545 | 0.6147 | 0.094* |
| C11 | 0.6698 (3) | 0.99895 (19) | 0.82931 (15) | 0.0626 (6) |
| C12 | 0.5408 (3) | 0.91601 (18) | 0.88072 (14) | 0.0600 (5) |
| H12 | 0.3940 | 0.8946 | 0.8695 | 0.072* |
| C13 | 0.6269 (3) | 0.86427 (19) | 0.94871 (15) | 0.0617 (5) |
| C14 | 0.5022 (3) | 0.77346 (18) | 1.00488 (14) | 0.0565 (5) |
| C15 | 0.2822 (3) | 0.73328 (18) | 0.99912 (15) | 0.0611 (5) |
| H15 | 0.2061 | 0.7648 | 0.9584 | 0.073* |
| C16 | 0.1744 (3) | 0.64730 (19) | 1.05277 (15) | 0.0619 (6) |
| H16 | 0.0265 | 0.6230 | 1.0485 | 0.074* |
| C17 | 0.2820 (3) | 0.59616 (18) | 1.11318 (14) | 0.0555 (5) |
| C18 | 0.5022 (3) | 0.6383 (2) | 1.11969 (16) | 0.0695 (6) |
| H18 | 0.5784 | 0.6070 | 1.1605 | 0.083* |
| C19 | 0.6108 (3) | 0.7254 (2) | 1.06730 (16) | 0.0689 (6) |
| H19 | 0.7585 | 0.7524 | 1.0737 | 0.083* |
| C20 | 0.1692 (3) | 0.50258 (18) | 1.17043 (14) | 0.0574 (5) |
| C21 | −0.0199 (3) | 0.5076 (2) | 1.21068 (17) | 0.0740 (6) |
| H21 | −0.0777 | 0.5713 | 1.2015 | 0.089* |
| C22 | −0.1241 (4) | 0.4204 (2) | 1.26393 (19) | 0.0876 (8) |
| H22 | −0.2509 | 0.4256 | 1.2903 | 0.105* |
| C23 | −0.0412 (4) | 0.3262 (2) | 1.27805 (18) | 0.0879 (8) |
| H23 | −0.1102 | 0.2680 | 1.3150 | 0.105* |
| C24 | 0.1417 (4) | 0.3177 (2) | 1.23808 (18) | 0.0884 (8) |
| H24 | 0.1961 | 0.2524 | 1.2466 | 0.106* |
| C25 | 0.2482 (4) | 0.4050 (2) | 1.18479 (16) | 0.0747 (7) |
| H25 | 0.3742 | 0.3982 | 1.1583 | 0.090* |
| O1 | 0.8736 (2) | 1.02827 (16) | 0.84284 (13) | 0.0910 (6) |
| O2 | 0.8298 (2) | 0.89287 (17) | 0.96452 (13) | 0.0948 (6) |
| H1 | 0.887 (4) | 0.966 (3) | 0.909 (2) | 0.142* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.161 (5) | 0.128 (4) | 0.103 (3) | 0.020 (3) | −0.031 (3) | 0.050 (3) |
| C2 | 0.187 (5) | 0.108 (3) | 0.113 (3) | 0.083 (4) | 0.009 (3) | 0.031 (3) |
| C3 | 0.130 (4) | 0.246 (7) | 0.120 (4) | 0.070 (4) | 0.055 (3) | 0.127 (5) |
| C1' | 0.103 (8) | 0.098 (9) | 0.108 (9) | 0.036 (7) | 0.007 (7) | 0.027 (7) |
| C2' | 0.149 (10) | 0.097 (8) | 0.126 (10) | 0.024 (7) | −0.007 (8) | 0.063 (8) |
| C3' | 0.153 (11) | 0.133 (10) | 0.080 (8) | 0.056 (8) | −0.001 (7) | 0.043 (7) |
| C4 | 0.1001 (18) | 0.0725 (15) | 0.0668 (16) | 0.0307 (14) | 0.0176 (13) | 0.0285 (13) |
| C5 | 0.0808 (15) | 0.0606 (13) | 0.0561 (13) | 0.0245 (11) | 0.0183 (11) | 0.0158 (11) |
| C6 | 0.0668 (14) | 0.0888 (17) | 0.0811 (17) | 0.0176 (12) | 0.0080 (12) | 0.0382 (14) |
| C7 | 0.0631 (14) | 0.0764 (15) | 0.0761 (16) | 0.0097 (11) | 0.0108 (11) | 0.0346 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.0660 (13) | 0.0561 (12) | 0.0521 (13) | 0.0149 (10) | 0.0106 (10) | 0.0111 (10) |
| C9 | 0.0665 (14) | 0.0820 (16) | 0.0796 (17) | 0.0128 (12) | 0.0138 (12) | 0.0299 (14) |
| C10 | 0.0806 (17) | 0.0782 (15) | 0.0780 (17) | 0.0142 (13) | 0.0244 (13) | 0.0345 (14) |
| C11 | 0.0619 (14) | 0.0594 (13) | 0.0622 (14) | 0.0120 (11) | 0.0009 (11) | 0.0076 (11) |
| C12 | 0.0613 (12) | 0.0597 (12) | 0.0579 (13) | 0.0128 (10) | 0.0039 (10) | 0.0142 (11) |
| C13 | 0.0595 (13) | 0.0615 (13) | 0.0588 (13) | 0.0089 (10) | −0.0013 (10) | 0.0100 (11) |
| C14 | 0.0636 (13) | 0.0574 (12) | 0.0495 (12) | 0.0196 (10) | −0.0017 (10) | 0.0081 (10) |
| C15 | 0.0610 (13) | 0.0606 (13) | 0.0637 (14) | 0.0161 (10) | −0.0084 (10) | 0.0197 (11) |
| C16 | 0.0541 (12) | 0.0675 (13) | 0.0671 (14) | 0.0170 (10) | −0.0015 (10) | 0.0206 (12) |
| C17 | 0.0619 (13) | 0.0592 (12) | 0.0491 (12) | 0.0236 (10) | 0.0003 (9) | 0.0089 (10) |
| C18 | 0.0625 (14) | 0.0919 (16) | 0.0677 (14) | 0.0329 (12) | 0.0038 (11) | 0.0337 (13) |
| C19 | 0.0579 (13) | 0.0850 (15) | 0.0700 (15) | 0.0241 (11) | 0.0029 (11) | 0.0248 (13) |
| C20 | 0.0653 (13) | 0.0621 (13) | 0.0481 (12) | 0.0229 (10) | 0.0000 (10) | 0.0106 (10) |
| C21 | 0.0718 (15) | 0.0766 (15) | 0.0821 (17) | 0.0280 (12) | 0.0105 (12) | 0.0254 (13) |
| C22 | 0.0848 (17) | 0.0919 (18) | 0.0937 (19) | 0.0264 (15) | 0.0245 (14) | 0.0341 (16) |
| C23 | 0.113 (2) | 0.0825 (17) | 0.0712 (17) | 0.0225 (15) | 0.0186 (15) | 0.0314 (14) |
| C24 | 0.124 (2) | 0.0828 (17) | 0.0775 (18) | 0.0476 (16) | 0.0210 (16) | 0.0357 (15) |
| C25 | 0.0949 (17) | 0.0795 (15) | 0.0662 (15) | 0.0428 (13) | 0.0163 (12) | 0.0274 (13) |
| O1 | 0.0634 (11) | 0.1048 (13) | 0.1033 (13) | 0.0045 (9) | −0.0041 (9) | 0.0489 (11) |
| O2 | 0.0619 (10) | 0.1084 (13) | 0.1079 (14) | −0.0043 (9) | −0.0178 (9) | 0.0530 (12) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C4 | 1.566 (4) | C9—C10 | 1.377 (3) |
| C1—H1A | 0.9600 | C9—H9 | 0.9300 |
| C1—H1B | 0.9600 | C10—H10 | 0.9300 |
| C1—H1C | 0.9600 | C11—O1 | 1.289 (2) |
| C2—C4 | 1.500 (4) | C11—C12 | 1.388 (3) |
| C2—H2A | 0.9600 | C12—C13 | 1.391 (3) |
| C2—H2B | 0.9600 | C12—H12 | 0.9300 |
| C2—H2C | 0.9600 | C13—O2 | 1.287 (2) |
| C3—C4 | 1.496 (3) | C13—C14 | 1.475 (3) |
| C3—H3A | 0.9600 | C14—C15 | 1.384 (3) |
| C3—H3B | 0.9600 | C14—C19 | 1.390 (3) |
| C3—H3C | 0.9600 | C15—C16 | 1.378 (3) |
| C1'—C4 | 1.484 (6) | C15—H15 | 0.9300 |
| C1'—H1'1 | 0.9600 | C16—C17 | 1.389 (3) |
| C1'—H1'2 | 0.9600 | C16—H16 | 0.9300 |
| C1'—H1'3 | 0.9600 | C17—C18 | 1.387 (3) |
| C2'—C4 | 1.541 (7) | C17—C20 | 1.479 (3) |
| C2'—H2'1 | 0.9600 | C18—C19 | 1.375 (3) |
| C2'—H2'2 | 0.9600 | C18—H18 | 0.9300 |
| C2'—H2'3 | 0.9600 | C19—H19 | 0.9300 |
| C3'—C4 | 1.484 (7) | C20—C21 | 1.384 (3) |
| C3'—H3'1 | 0.9600 | C20—C25 | 1.387 (3) |
| C3'—H3'2 | 0.9600 | C21—C22 | 1.375 (3) |
| C3'—H3'3 | 0.9600 | C21—H21 | 0.9300 |
| C4—C5 | 1.534 (3) | C22—C23 | 1.365 (3) |
| C5—C10 | 1.371 (3) | C22—H22 | 0.9300 |

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| C5—C6 | 1.375 (3) | C23—C24 | 1.355 (3) |
| C6—C7 | 1.380 (3) | C23—H23 | 0.9300 |
| C6—H6 | 0.9300 | C24—C25 | 1.381 (3) |
| C7—C8 | 1.378 (3) | C24—H24 | 0.9300 |
| C7—H7 | 0.9300 | C25—H25 | 0.9300 |
| C8—C9 | 1.370 (3) | O1—H1 | 1.28 (4) |
| C8—C11 | 1.477 (3) | O2—H1 | 1.21 (3) |
| C4—C1—H1A | 109.5 | C9—C8—C7 | 117.1 (2) |
| C4—C1—H1B | 109.5 | C9—C8—C11 | 119.3 (2) |
| C4—C1—H1C | 109.5 | C7—C8—C11 | 123.53 (18) |
| C4—C2—H2A | 109.5 | C8—C9—C10 | 121.4 (2) |
| C4—C2—H2B | 109.5 | C8—C9—H9 | 119.3 |
| C4—C2—H2C | 109.5 | C10—C9—H9 | 119.3 |
| C4—C3—H3A | 109.5 | C5—C10—C9 | 122.1 (2) |
| C4—C3—H3B | 109.5 | C5—C10—H10 | 119.0 |
| C4—C3—H3C | 109.5 | C9—C10—H10 | 119.0 |
| C4—C1'—H1'1 | 109.5 | O1—C11—C12 | 120.27 (19) |
| C4—C1'—H1'2 | 109.5 | O1—C11—C8 | 115.13 (19) |
| H1'1—C1'—H1'2 | 109.5 | C12—C11—C8 | 124.6 (2) |
| C4—C1'—H1'3 | 109.5 | C11—C12—C13 | 121.2 (2) |
| H1'1—C1'—H1'3 | 109.5 | C11—C12—H12 | 119.4 |
| H1'2—C1'—H1'3 | 109.5 | C13—C12—H12 | 119.4 |
| C4—C2'—H2'1 | 109.5 | O2—C13—C12 | 119.88 (19) |
| C4—C2'—H2'2 | 109.5 | O2—C13—C14 | 115.25 (19) |
| H2'1—C2'—H2'2 | 109.5 | C12—C13—C14 | 124.85 (19) |
| C4—C2'—H2'3 | 109.5 | C15—C14—C19 | 117.93 (19) |
| H2'1—C2'—H2'3 | 109.5 | C15—C14—C13 | 123.62 (18) |
| H2'2—C2'—H2'3 | 109.5 | C19—C14—C13 | 118.45 (19) |
| C4—C3'—H3'1 | 109.5 | C16—C15—C14 | 121.01 (18) |
| C4—C3'—H3'2 | 109.5 | C16—C15—H15 | 119.5 |
| H3'1—C3'—H3'2 | 109.5 | C14—C15—H15 | 119.5 |
| C4—C3'—H3'3 | 109.5 | C15—C16—C17 | 121.36 (18) |
| H3'1—C3'—H3'3 | 109.5 | C15—C16—H16 | 119.3 |
| H3'2—C3'—H3'3 | 109.5 | C17—C16—H16 | 119.3 |
| C3'—C4—C1' | 113.2 (6) | C18—C17—C16 | 117.25 (18) |
| C3'—C4—C3 | 51.7 (6) | C18—C17—C20 | 120.55 (17) |
| C1'—C4—C3 | 131.9 (6) | C16—C17—C20 | 122.18 (18) |
| C3'—C4—C2 | 147.5 (6) | C19—C18—C17 | 121.67 (19) |
| C1'—C4—C2 | 52.3 (5) | C19—C18—H18 | 119.2 |
| C3—C4—C2 | 112.4 (3) | C17—C18—H18 | 119.2 |
| C3'—C4—C5 | 104.4 (6) | C18—C19—C14 | 120.7 (2) |
| C1'—C4—C5 | 114.6 (6) | C18—C19—H19 | 119.6 |
| C3—C4—C5 | 113.5 (2) | C14—C19—H19 | 119.6 |
| C2—C4—C5 | 108.1 (2) | C21—C20—C25 | 117.32 (19) |
| C3'—C4—C2' | 109.7 (6) | C21—C20—C17 | 121.70 (18) |
| C1'—C4—C2' | 109.1 (5) | C25—C20—C17 | 120.97 (18) |
| C3—C4—C2' | 58.2 (6) | C22—C21—C20 | 121.5 (2) |
| C2—C4—C2' | 60.9 (6) | C22—C21—H21 | 119.3 |
| C5—C4—C2' | 105.5 (5) | C20—C21—H21 | 119.3 |

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| C3'—C4—C1 | 62.0 (6) | C23—C22—C21 | 120.0 (2) |
| C1'—C4—C1 | 54.5 (6) | C23—C22—H22 | 120.0 |
| C3—C4—C1 | 106.2 (3) | C21—C22—H22 | 120.0 |
| C2—C4—C1 | 105.8 (3) | C24—C23—C22 | 119.8 (2) |
| C5—C4—C1 | 110.6 (2) | C24—C23—H23 | 120.1 |
| C2'—C4—C1 | 143.9 (5) | C22—C23—H23 | 120.1 |
| C10—C5—C6 | 116.3 (2) | C23—C24—C25 | 120.7 (2) |
| C10—C5—C4 | 121.3 (2) | C23—C24—H24 | 119.7 |
| C6—C5—C4 | 122.3 (2) | C25—C24—H24 | 119.7 |
| C5—C6—C7 | 122.0 (2) | C24—C25—C20 | 120.7 (2) |
| C5—C6—H6 | 119.0 | C24—C25—H25 | 119.7 |
| C7—C6—H6 | 119.0 | C20—C25—H25 | 119.7 |
| C8—C7—C6 | 121.00 (19) | C11—O1—H1 | 99.3 (13) |
| C8—C7—H7 | 119.5 | C13—O2—H1 | 100.4 (14) |
| C6—C7—H7 | 119.5 | | |
| C3'—C4—C5—C10 | 82.9 (7) | C11—C12—C13—O2 | −0.3 (3) |
| C1'—C4—C5—C10 | −152.7 (7) | C11—C12—C13—C14 | −178.54 (17) |
| C3—C4—C5—C10 | 28.8 (4) | O2—C13—C14—C15 | 178.66 (19) |
| C2—C4—C5—C10 | −96.6 (3) | C12—C13—C14—C15 | −3.0 (3) |
| C2'—C4—C5—C10 | −32.8 (7) | O2—C13—C14—C19 | −1.2 (3) |
| C1—C4—C5—C10 | 148.0 (3) | C12—C13—C14—C19 | 177.1 (2) |
| C3'—C4—C5—C6 | −98.9 (7) | C19—C14—C15—C16 | −0.7 (3) |
| C1'—C4—C5—C6 | 25.5 (7) | C13—C14—C15—C16 | 179.40 (19) |
| C3—C4—C5—C6 | −153.0 (3) | C14—C15—C16—C17 | −1.2 (3) |
| C2—C4—C5—C6 | 81.6 (3) | C15—C16—C17—C18 | 2.1 (3) |
| C2'—C4—C5—C6 | 145.4 (7) | C15—C16—C17—C20 | −179.21 (18) |
| C1—C4—C5—C6 | −33.8 (3) | C16—C17—C18—C19 | −1.3 (3) |
| C10—C5—C6—C7 | −1.1 (3) | C20—C17—C18—C19 | −179.93 (19) |
| C4—C5—C6—C7 | −179.4 (2) | C17—C18—C19—C14 | −0.6 (3) |
| C5—C6—C7—C8 | −0.9 (4) | C15—C14—C19—C18 | 1.6 (3) |
| C6—C7—C8—C9 | 2.0 (3) | C13—C14—C19—C18 | −178.52 (19) |
| C6—C7—C8—C11 | −178.2 (2) | C18—C17—C20—C21 | 142.2 (2) |
| C7—C8—C9—C10 | −1.1 (3) | C16—C17—C20—C21 | −36.4 (3) |
| C11—C8—C9—C10 | 179.1 (2) | C18—C17—C20—C25 | −38.7 (3) |
| C6—C5—C10—C9 | 2.0 (3) | C16—C17—C20—C25 | 142.7 (2) |
| C4—C5—C10—C9 | −179.7 (2) | C25—C20—C21—C22 | 0.9 (3) |
| C8—C9—C10—C5 | −0.9 (4) | C17—C20—C21—C22 | −179.9 (2) |
| C9—C8—C11—O1 | −2.2 (3) | C20—C21—C22—C23 | 0.0 (4) |
| C7—C8—C11—O1 | 178.0 (2) | C21—C22—C23—C24 | −1.2 (4) |
| C9—C8—C11—C12 | 178.42 (19) | C22—C23—C24—C25 | 1.4 (4) |
| C7—C8—C11—C12 | −1.4 (3) | C23—C24—C25—C20 | −0.5 (4) |
| O1—C11—C12—C13 | 1.0 (3) | C21—C20—C25—C24 | −0.6 (3) |
| C8—C11—C12—C13 | −179.59 (19) | C17—C20—C25—C24 | −179.8 (2) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O2 | 1.28 (3) | 1.22 (3) | 2.453 (3) | 159 (3) |
| O1—H1···O2$^{i}$ | 1.28 (4) | 2.56 (3) | 3.183 (2) | 107.1 (17) |

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*+2.

**Fig. 1**