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4-Hydroxy-4,6a,6b,9,9,12a,14b-heptamethylperhydropicen-3-one hemihydrate isolated from *Adiantum incisum*

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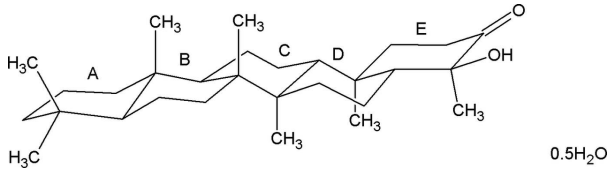
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.011 Å; H-atom completeness 98%; R factor = 0.071; wR factor = 0.147; data-to-parameter ratio = 6.4.

The title compound, $C_{29}H_{48}O_2\cdot0.5H_2O$, is a triterpenoid isolated from the stems and rhizomes of *Adiantum incisum*. The basic skeleton of the molecule contains five six-membered rings, all adopting chair conformations, bearing a total of seven methyl, one hydroxyl and a keto group. There are two molecules of the triterpene and one water molecule of crystallization in the asymmetric unit. The two unique triterpenoid molecules hydrogen-bond directly *via* an O—H···O=C interaction, and are also bridged by the water molecule. The water also bridges to another pair of hydrogen-bonded triterpenoid molecules.

Related literature

For related literature, see: Ageta *et al.* (1966); Janaki *et al.* (1999); Kshirsagar & Mehta (1972); Matsuda *et al.* (1999); Wada *et al.* (1987).



Experimental

Crystal data

$C_{29}H_{48}O_2\cdot0.5H_2O$
M_r = 437.68
Monoclinic, $P2_1$
a = 6.4432 (4) Å
b = 57.477 (8) Å
c = 7.2226 (6) Å
β = 114.725 (5)°
V = 2429.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 120 (2) K
0.42 × 0.20 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.970, T_{max} = 0.996
12411 measured reflections
3758 independent reflections
2285 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.147
S = 1.05
3758 reflections
584 parameters
52 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O4	0.84	2.19	2.978 (8)	156
O3—H3···O5	0.84	2.06	2.896 (9)	176

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2638).

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4-Hydroxy-4,6a,6b,9,9,12a,14b-heptamethylperhydropicen-3-one hemihydrate isolated from *Adiantum incisum*

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S1. Comment

Triterpenoids represent an important class of natural products characterized by highly pronounced biological activities such as analgesic, anti-mutagenic, and anti-inflammatory (Matsuda *et al.* 1999; Janaki *et al.* 1999). *Adiantum incisum,* a fern, generally found in the Himalayas region is well known for its antibacterial, antiviral and antifungal activities (Kshirsagar *et al.* 1972; Wada *et al.* 1987). The plant for the present work was collected from the Murree hills of Pakistan and during its phytochemical investigations, title compound (**I**) was isolated and its crystal structure is being reported here for the first time. (**I**) has also been reported as one of the constituents of *Adiantum monochlamys* (Ageta *et al.* 1966).

The molecule (**I**) is shown in Fig.1 and contains five six membered rings, all adopting chair conformations, fused together in a *trans* fashion. All the rings at their juncture bear one methyl group while ring A has two extra methyl groups. Ring E is in a slightly distorted form due to the presence of one methyl and a hydroxyl group at one carbon, C1, and a keto group on the adjacent carbon, C2.

The arrangement of molecular units suggests that the three dimensional structure is stabilized by inter molecular hydrogen bonds. Carbonyl oxygen (O4) of one triterpenoid molecule is involved in hydrogen bonding with the hydroxyl hydrogen (H1) of the other while its hydroxyl hydrogen (H3) is H-bonded with the oxygen (O5) of the water molecule. The H atoms of the water molecule are involved in inter-molecular hydrogen bonding with hydroxyl oxygen O1 (O1···O5 = 3.009 (9) Å) and carbonyl oxygen O2i (O5···O2i = 2.834 (9) Å; symmetry operator i = x + 1, y, z + 1) of the adjacent pair of molecules making an infinite chain along [1 0 1] as shown in Figs 2 & 3.

S2. Experimental

The plant (*Adiantum incisum)* collected from Murree hills, Pakistan, was shade dried. The dried stems and rhizomes (2.9 kg) were dipped in ethanol for fifteen days and filtered. The filtrate was concentrated under reduced pressure to obtain the extract (51.33 g) followed by column chromatography using a gradient solvent system from hexane-chloroform-methanol. The eluted fractions were monitored by thin layer chromatography and combined to give 38 main fractions. Fraction 9 was rechromatographed on a silica-gel column with hexane-chloroform (1:1) to afford the pure title compound (**I**).

S3. Refinement

In the absence of anomalous scatterers Friedel pairs were merged and the absolute configuration of the compound was arbitrarily set. H atoms bound to C were placed in geometric positions (C—H distance = 0.99 Å for methylene; 1.00 Å for methyl H; 0.84 Å for OH) using a riding model. H atoms on the water molecules were not located in difference maps or included in the model. U_{iso} values were set to 1.2U_{eq} (1.5U_{eq} for methyl H and O*H*) of the carrier atom. The

displacement parameters of the atoms C33 C36, C48, C51 and C53 were restrained to an isotropic behaviour.

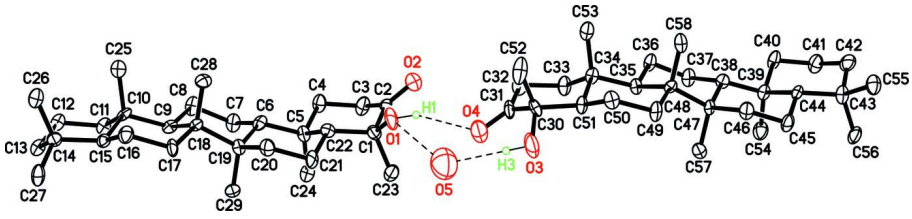

Figure 1

Asymmetric unit of (**I**). Displacement ellipsoids are drawn at the 50% probability level, H atoms are represented by circles of arbitrary radius and hydrogen bonds are shown as dashed lines.

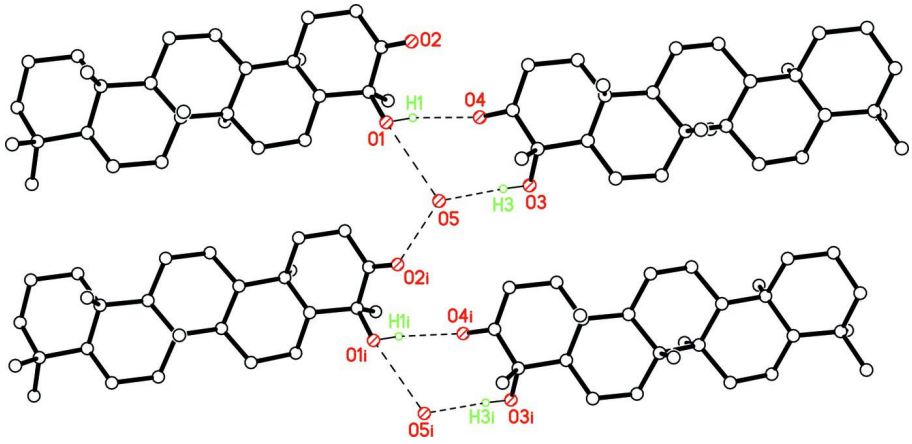

Figure 2

Close-up of the H-bonding motif in (**I**) showing showing the arrangement of three triterpenoid molecules H-bonded through one water molecule. Symmetry operator: i = $x + 1$, y, $z + 1$.

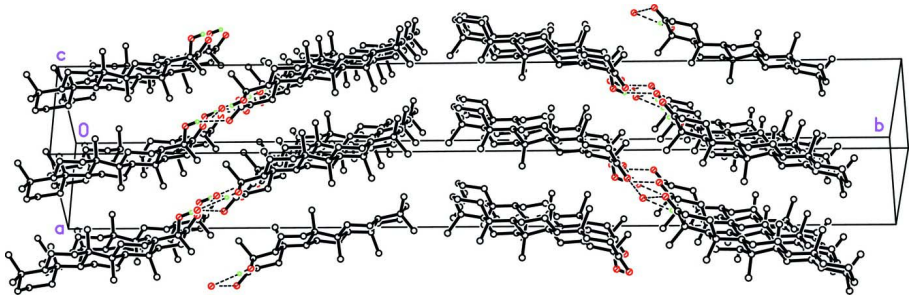

Figure 3

Packing plot of (**I**) viewed approximately along the chain propagation direction [1 0 1].

4-Hydroxy-4,6a,6 b,9,9,12a,14*b*-heptamethylperhydropicen-3-one hemihydrate

Crystal data

$C_{29}H_{48}O_2 \cdot 0.5H_2O$
$M_r = 437.68$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 6.4432$ (4) Å
$b = 57.477$ (8) Å
$c = 7.2226$ (6) Å
$\beta = 114.725$ (5)°
$V = 2429.6$ (4) Å^3
$Z = 4$
$F(000) = 972$
$D_x = 1.197$ Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 10245 reflections
θ = 1.0–27.5°
μ = 0.07 mm^{-1}
T = 120 K
Plate, colourless
0.42 × 0.20 × 0.06 mm

Data collection

Bruker–Nonius Kappa CCD diffractometer
Radiation source: Bruker-Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ & ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.970, T_{max} = 0.996
12411 measured reflections
3758 independent reflections
2285 reflections with $I > 2\sigma(I)$
R_{int} = 0.064
θ_{max} = 25.0°, θ_{min} = 5.0°
h = −7→7
k = −68→68
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.147
S = 1.05
3758 reflections
584 parameters
52 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
$w = 1/[\sigma^2(F_o^2) + (0.0174P)^2 + 4.4271P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 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. Flack gave no indication of absolute structure, so Friedels merged. Material isolated from a plant, but no clear idea of absolute structure. Most likely this is correct however.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.9141 (13)	0.15886 (12)	0.0149 (12)	0.0246 (19)
O1	0.8628 (10)	0.16278 (9)	0.1878 (9)	0.0382 (16)
H1	0.8052	0.1761	0.1792	0.057*
C2	0.7039 (13)	0.16394 (12)	−0.1775 (13)	0.027 (2)
O2	0.5468 (10)	0.17554 (9)	−0.1680 (9)	0.0424 (16)
C3	0.6946 (15)	0.15411 (12)	−0.3734 (13)	0.034 (2)
H3A	0.8056	0.1625	−0.4114	0.041*
H3B	0.5401	0.1566	−0.4832	0.041*
C4	0.7496 (14)	0.12804 (12)	−0.3550 (12)	0.028 (2)
H4A	0.7565	0.1226	−0.4825	0.034*

H4B	0.6242	0.1195	−0.3397	0.034*
C5	0.9782 (13)	0.12198 (12)	−0.1726 (11)	0.0199 (18)
C6	0.9908 (13)	0.09486 (11)	−0.1440 (12)	0.0223 (19)
H6	0.8464	0.0904	−0.1328	0.027*
C7	0.9876 (14)	0.08129 (12)	−0.3270 (12)	0.027 (2)
H7A	1.1312	0.0844	−0.3415	0.033*
H7B	0.8593	0.0869	−0.4521	0.033*
C8	0.9619 (14)	0.05492 (12)	−0.3079 (12)	0.027 (2)
H8A	0.8092	0.0517	−0.3121	0.032*
H8B	0.9715	0.0470	−0.4259	0.032*
C9	1.1456 (12)	0.04490 (11)	−0.1102 (11)	0.0191 (18)
H9	1.2947	0.0493	−0.1123	0.023*
C10	1.1479 (12)	0.01764 (11)	−0.1013 (11)	0.0171 (18)
C11	1.2009 (13)	0.00819 (12)	−0.2769 (11)	0.0231 (19)
H11A	1.0692	0.0115	−0.4080	0.028*
H11B	1.3349	0.0166	−0.2772	0.028*
C12	1.2498 (13)	−0.01789 (12)	−0.2628 (11)	0.0234 (19)
H12A	1.1109	−0.0265	−0.2767	0.028*
H12B	1.2885	−0.0226	−0.3763	0.028*
C13	1.4462 (13)	−0.02423 (12)	−0.0607 (11)	0.0239 (19)
H13A	1.5889	−0.0174	−0.0573	0.029*
H13B	1.4646	−0.0413	−0.0538	0.029*
C14	1.4153 (13)	−0.01598 (12)	0.1279 (12)	0.0228 (19)
C15	1.3517 (13)	0.01046 (11)	0.1021 (11)	0.0202 (18)
H15	1.4879	0.0183	0.0976	0.024*
C16	1.3269 (14)	0.02130 (12)	0.2849 (13)	0.028 (2)
H16A	1.4545	0.0161	0.4124	0.034*
H16B	1.1821	0.0160	0.2879	0.034*
C17	1.3279 (13)	0.04789 (11)	0.2727 (12)	0.025 (2)
H17A	1.4785	0.0530	0.2815	0.030*
H17B	1.3096	0.0544	0.3920	0.030*
C18	1.1388 (12)	0.05814 (11)	0.0761 (12)	0.0178 (18)
C19	1.1891 (12)	0.08532 (12)	0.0555 (11)	0.0174 (18)
C20	1.1912 (14)	0.09901 (12)	0.2401 (12)	0.027 (2)
H20A	1.3310	0.0949	0.3622	0.032*
H20B	1.0579	0.0942	0.2656	0.032*
C21	1.1839 (14)	0.12576 (11)	0.2096 (12)	0.026 (2)
H21A	1.1798	0.1336	0.3301	0.031*
H21B	1.3230	0.1309	0.1953	0.031*
C22	0.9710 (13)	0.13238 (12)	0.0179 (11)	0.0207 (18)
H22	0.8418	0.1242	0.0330	0.025*
C23	1.1030 (13)	0.17568 (12)	0.0279 (13)	0.034 (2)
H23A	1.0559	0.1917	0.0383	0.051*
H23B	1.1314	0.1742	−0.0947	0.051*
H23C	1.2432	0.1720	0.1485	0.051*
C24	1.1701 (13)	0.13176 (12)	−0.2263 (11)	0.0236 (19)
H24A	1.1163	0.1460	−0.3077	0.035*
H24B	1.2110	0.1201	−0.3047	0.035*

H24C	1.3045	0.1354	−0.1005	0.035*
C25	0.9171 (12)	0.00745 (12)	−0.1252 (12)	0.0259 (19)
H25A	0.7927	0.0173	−0.2172	0.039*
H25B	0.9118	0.0068	0.0083	0.039*
H25C	0.8998	−0.0083	−0.1820	0.039*
C26	1.2423 (14)	−0.03148 (13)	0.1681 (13)	0.031 (2)
H26A	1.1008	−0.0327	0.0434	0.046*
H26B	1.2090	−0.0246	0.2768	0.046*
H26C	1.3075	−0.0470	0.2098	0.046*
C27	1.6484 (14)	−0.01867 (13)	0.3106 (12)	0.030 (2)
H27A	1.7076	−0.0344	0.3105	0.045*
H27B	1.6307	−0.0162	0.4374	0.045*
H27C	1.7555	−0.0072	0.3002	0.045*
C28	0.9116 (12)	0.05487 (12)	0.0917 (12)	0.0238 (19)
H28A	0.8950	0.0385	0.1222	0.036*
H28B	0.7859	0.0592	−0.0380	0.036*
H28C	0.9081	0.0648	0.2007	0.036*
C29	1.4230 (12)	0.08909 (12)	0.0534 (13)	0.029 (2)
H29A	1.4168	0.0844	−0.0792	0.043*
H29B	1.5376	0.0797	0.1611	0.043*
H29C	1.4644	0.1056	0.0771	0.043*
C30	0.6577 (13)	0.23570 (13)	0.3874 (12)	0.0249 (19)
O3	0.8893 (10)	0.23628 (10)	0.5368 (10)	0.0515 (18)
H3	0.9512	0.2233	0.5399	0.077*
C31	0.6470 (14)	0.22709 (12)	0.1855 (13)	0.029 (2)
O4	0.8017 (11)	0.21414 (11)	0.1883 (11)	0.0571 (19)
C32	0.4497 (15)	0.23372 (13)	−0.0082 (13)	0.036 (2)
H32A	0.3154	0.2242	−0.0240	0.043*
H32B	0.4879	0.2302	−0.1246	0.043*
C33	0.3868 (14)	0.25972 (12)	−0.0144 (12)	0.0275 (18)
H33A	0.2433	0.2627	−0.1367	0.033*
H33B	0.5086	0.2692	−0.0267	0.033*
C34	0.3552 (13)	0.26759 (12)	0.1794 (11)	0.0187 (15)
C35	0.3424 (13)	0.29505 (11)	0.1735 (11)	0.0173 (15)
H35	0.4811	0.3003	0.1561	0.021*
C36	0.1399 (13)	0.30474 (11)	−0.0097 (12)	0.0239 (18)
H36A	−0.0029	0.3008	0.0035	0.029*
H36B	0.1339	0.2972	−0.1350	0.029*
C37	0.1517 (14)	0.33131 (12)	−0.0317 (12)	0.026 (2)
H37A	0.2804	0.3351	−0.0675	0.031*
H37B	0.0091	0.3367	−0.1449	0.031*
C38	0.1835 (13)	0.34441 (11)	0.1616 (11)	0.0205 (19)
H38	0.0482	0.3400	0.1881	0.025*
C39	0.1706 (13)	0.37191 (12)	0.1389 (11)	0.0182 (18)
C40	−0.0682 (13)	0.37832 (12)	−0.0267 (12)	0.028 (2)
H40A	−0.0795	0.3730	−0.1609	0.034*
H40B	−0.1861	0.3700	0.0018	0.034*
C41	−0.1181 (14)	0.40456 (12)	−0.0376 (13)	0.033 (2)

H41A	−0.2746	0.4076	−0.1420	0.040*
H41B	−0.0093	0.4130	−0.0778	0.040*
C42	−0.0955 (14)	0.41349 (13)	0.1714 (13)	0.036 (2)
H42A	−0.1224	0.4305	0.1625	0.043*
H42B	−0.2156	0.4061	0.2033	0.043*
C43	0.1355 (13)	0.40857 (12)	0.3442 (12)	0.024 (2)
C44	0.1912 (13)	0.38201 (12)	0.3461 (12)	0.0216 (19)
H44	0.0688	0.3740	0.3728	0.026*
C45	0.4146 (13)	0.37456 (12)	0.5217 (12)	0.027 (2)
H45A	0.4274	0.3820	0.6497	0.033*
H45B	0.5456	0.3798	0.4944	0.033*
C46	0.4217 (14)	0.34792 (12)	0.5456 (12)	0.027 (2)
H46A	0.2976	0.3431	0.5840	0.033*
H46B	0.5687	0.3435	0.6582	0.033*
C47	0.3952 (12)	0.33463 (11)	0.3490 (11)	0.0167 (17)
C48	0.3570 (12)	0.30739 (11)	0.3748 (11)	0.0161 (16)
C49	0.5583 (13)	0.29709 (11)	0.5616 (11)	0.024 (2)
H49A	0.7033	0.3030	0.5631	0.029*
H49B	0.5479	0.3027	0.6871	0.029*
C50	0.5657 (14)	0.27055 (12)	0.5658 (11)	0.0236 (19)
H50A	0.4286	0.2644	0.5781	0.028*
H50B	0.7026	0.2652	0.6852	0.028*
C51	0.5737 (13)	0.26148 (11)	0.3691 (11)	0.0200 (16)
H51	0.6969	0.2708	0.3541	0.024*
C52	0.5191 (16)	0.21872 (13)	0.4547 (14)	0.045 (3)
H52A	0.5911	0.2033	0.4783	0.067*
H52B	0.3632	0.2176	0.3479	0.067*
H52C	0.5145	0.2244	0.5810	0.067*
C53	0.1367 (13)	0.25633 (12)	0.1725 (13)	0.0317 (19)
H53A	0.1262	0.2403	0.1236	0.048*
H53B	0.0036	0.2652	0.0800	0.048*
H53C	0.1404	0.2563	0.3096	0.048*
C54	0.3513 (14)	0.38123 (13)	0.0706 (13)	0.035 (2)
H54A	0.3017	0.3963	0.0035	0.052*
H54B	0.3699	0.3702	−0.0250	0.052*
H54C	0.4973	0.3831	0.1899	0.052*
C55	0.1109 (14)	0.41428 (13)	0.5426 (13)	0.032 (2)
H55A	0.0353	0.4294	0.5286	0.048*
H55B	0.2626	0.4149	0.6564	0.048*
H55C	0.0191	0.4022	0.5687	0.048*
C56	0.3179 (13)	0.42516 (12)	0.3354 (13)	0.032 (2)
H56A	0.2803	0.4412	0.3566	0.048*
H56B	0.3223	0.4239	0.2018	0.048*
H56C	0.4675	0.4210	0.4423	0.048*
C57	0.6213 (13)	0.33865 (12)	0.3247 (13)	0.028 (2)
H57A	0.5946	0.3360	0.1824	0.042*
H57B	0.7382	0.3278	0.4129	0.042*
H57C	0.6735	0.3547	0.3633	0.042*

C58	0.1398 (13)	0.30336 (12)	0.4067 (13)	0.029 (2)
H58A	0.1397	0.2874	0.4553	0.044*
H58B	0.0058	0.3056	0.2774	0.044*
H58C	0.1346	0.3144	0.5080	0.044*
O5	1.1056 (14)	0.19142 (14)	0.5664 (13)	0.094 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.022 (5)	0.026 (4)	0.025 (5)	0.003 (3)	0.009 (4)	−0.003 (4)
O1	0.055 (4)	0.029 (3)	0.046 (4)	0.014 (3)	0.036 (3)	−0.002 (3)
C2	0.017 (5)	0.012 (4)	0.048 (6)	−0.001 (3)	0.009 (4)	0.008 (4)
O2	0.036 (4)	0.034 (3)	0.056 (5)	0.006 (3)	0.017 (3)	0.002 (3)
C3	0.042 (6)	0.022 (4)	0.028 (6)	0.001 (4)	0.004 (4)	0.000 (4)
C4	0.038 (5)	0.022 (4)	0.020 (5)	0.004 (4)	0.007 (4)	0.001 (4)
C5	0.028 (5)	0.021 (4)	0.011 (5)	0.006 (3)	0.009 (4)	0.004 (3)
C6	0.032 (5)	0.019 (4)	0.021 (5)	−0.005 (3)	0.017 (4)	0.002 (3)
C7	0.037 (5)	0.025 (4)	0.012 (5)	0.004 (4)	0.003 (4)	0.003 (4)
C8	0.046 (5)	0.022 (4)	0.015 (5)	0.002 (4)	0.016 (4)	0.004 (3)
C9	0.025 (4)	0.023 (4)	0.014 (5)	−0.005 (3)	0.013 (4)	0.001 (3)
C10	0.024 (4)	0.018 (4)	0.009 (5)	−0.009 (3)	0.007 (4)	0.002 (3)
C11	0.034 (5)	0.021 (4)	0.013 (5)	−0.004 (3)	0.009 (4)	−0.002 (3)
C12	0.038 (5)	0.021 (4)	0.019 (5)	−0.003 (4)	0.020 (4)	−0.002 (4)
C13	0.033 (5)	0.021 (4)	0.019 (5)	−0.004 (3)	0.013 (4)	−0.001 (3)
C14	0.021 (5)	0.023 (4)	0.021 (5)	−0.001 (3)	0.006 (4)	−0.003 (4)
C15	0.022 (4)	0.019 (4)	0.022 (5)	−0.002 (3)	0.012 (4)	0.000 (3)
C16	0.035 (5)	0.023 (4)	0.030 (6)	0.000 (4)	0.017 (4)	0.004 (4)
C17	0.034 (5)	0.015 (4)	0.033 (6)	0.007 (3)	0.021 (4)	0.000 (4)
C18	0.018 (4)	0.017 (4)	0.016 (5)	−0.003 (3)	0.006 (4)	0.001 (3)
C19	0.026 (5)	0.021 (4)	0.007 (5)	0.003 (3)	0.010 (4)	−0.003 (3)
C20	0.028 (5)	0.025 (4)	0.021 (5)	0.004 (4)	0.006 (4)	0.002 (4)
C21	0.038 (5)	0.020 (4)	0.026 (5)	0.001 (4)	0.020 (4)	−0.010 (3)
C22	0.022 (5)	0.025 (4)	0.017 (5)	0.000 (3)	0.010 (4)	−0.001 (3)
C23	0.037 (5)	0.023 (4)	0.045 (6)	−0.005 (4)	0.021 (5)	−0.005 (4)
C24	0.039 (5)	0.023 (4)	0.010 (5)	0.000 (3)	0.011 (4)	0.004 (3)
C25	0.033 (5)	0.026 (4)	0.018 (5)	0.002 (4)	0.011 (4)	0.002 (4)
C26	0.040 (5)	0.022 (4)	0.029 (6)	0.001 (4)	0.014 (5)	0.003 (4)
C27	0.046 (6)	0.018 (4)	0.021 (5)	0.005 (4)	0.010 (4)	−0.004 (4)
C28	0.025 (5)	0.029 (4)	0.024 (5)	−0.004 (3)	0.017 (4)	−0.005 (4)
C29	0.024 (5)	0.024 (4)	0.044 (6)	−0.003 (3)	0.018 (4)	0.002 (4)
C30	0.029 (5)	0.026 (4)	0.025 (5)	0.012 (4)	0.016 (4)	0.000 (4)
O3	0.050 (4)	0.035 (3)	0.056 (5)	0.024 (3)	0.009 (4)	−0.005 (3)
C31	0.040 (6)	0.016 (4)	0.037 (6)	0.007 (4)	0.023 (5)	−0.002 (4)
O4	0.059 (5)	0.038 (4)	0.086 (6)	0.009 (3)	0.041 (4)	−0.002 (4)
C32	0.055 (6)	0.028 (4)	0.029 (6)	0.000 (4)	0.022 (5)	0.000 (4)
C33	0.043 (5)	0.024 (4)	0.015 (4)	0.005 (4)	0.011 (4)	−0.002 (3)
C34	0.030 (4)	0.018 (3)	0.006 (4)	0.002 (3)	0.005 (3)	0.002 (3)
C35	0.024 (4)	0.020 (3)	0.004 (4)	0.004 (3)	0.003 (3)	−0.002 (3)

C36	0.031 (4)	0.017 (4)	0.014 (4)	0.003 (3)	−0.001 (3)	−0.001 (3)
C37	0.031 (5)	0.026 (4)	0.009 (5)	0.006 (4)	−0.004 (4)	−0.005 (3)
C38	0.019 (4)	0.020 (4)	0.014 (5)	0.004 (3)	−0.001 (4)	0.002 (3)
C39	0.026 (5)	0.020 (4)	0.006 (5)	0.000 (3)	0.005 (4)	−0.001 (3)
C40	0.035 (5)	0.018 (4)	0.016 (5)	0.004 (4)	−0.005 (4)	−0.002 (3)
C41	0.036 (5)	0.024 (4)	0.028 (6)	0.006 (4)	0.002 (4)	0.000 (4)
C42	0.033 (5)	0.019 (4)	0.051 (7)	−0.001 (4)	0.013 (5)	0.003 (4)
C43	0.038 (5)	0.019 (4)	0.014 (5)	0.005 (4)	0.011 (4)	0.002 (3)
C44	0.024 (4)	0.013 (4)	0.027 (5)	−0.003 (3)	0.009 (4)	−0.004 (3)
C45	0.031 (5)	0.021 (4)	0.021 (5)	0.000 (3)	0.003 (4)	−0.007 (4)
C46	0.027 (5)	0.024 (4)	0.021 (5)	0.005 (3)	0.000 (4)	−0.002 (3)
C47	0.022 (4)	0.018 (4)	0.006 (5)	0.003 (3)	0.001 (4)	−0.005 (3)
C48	0.017 (4)	0.019 (3)	0.008 (4)	−0.003 (3)	0.001 (3)	−0.003 (3)
C49	0.038 (5)	0.021 (4)	0.007 (5)	0.005 (4)	0.003 (4)	−0.005 (3)
C50	0.031 (5)	0.028 (4)	0.010 (5)	0.005 (4)	0.006 (4)	0.001 (3)
C51	0.034 (4)	0.016 (3)	0.012 (4)	0.003 (3)	0.012 (3)	−0.001 (3)
C52	0.082 (8)	0.021 (4)	0.036 (6)	0.007 (5)	0.030 (6)	0.002 (4)
C53	0.038 (4)	0.021 (4)	0.035 (6)	0.002 (3)	0.014 (4)	−0.002 (4)
C54	0.048 (6)	0.024 (4)	0.041 (6)	−0.003 (4)	0.028 (5)	0.000 (4)
C55	0.046 (6)	0.023 (4)	0.033 (6)	0.003 (4)	0.022 (5)	0.002 (4)
C56	0.038 (5)	0.016 (4)	0.039 (6)	−0.004 (4)	0.014 (5)	−0.004 (4)
C57	0.027 (5)	0.025 (4)	0.033 (6)	0.003 (4)	0.015 (4)	−0.001 (4)
C58	0.037 (5)	0.020 (4)	0.030 (6)	0.008 (4)	0.014 (4)	−0.001 (4)
O5	0.109 (7)	0.076 (5)	0.115 (7)	0.010 (5)	0.065 (6)	0.010 (5)

Geometric parameters (Å, º)

C1—O1	1.437 (9)	C30—O3	1.430 (9)
C1—C2	1.509 (11)	C30—C31	1.514 (11)
C1—C23	1.526 (10)	C30—C52	1.533 (11)
C1—C22	1.563 (10)	C30—C51	1.564 (10)
O1—H1	0.8400	O3—H3	0.8400
C2—O2	1.238 (9)	C31—O4	1.238 (9)
C2—C3	1.501 (11)	C31—C32	1.494 (11)
C3—C4	1.533 (10)	C32—C33	1.544 (10)
C3—H3A	0.9900	C32—H32A	0.9900
C3—H3B	0.9900	C32—H32B	0.9900
C4—C5	1.550 (10)	C33—C34	1.563 (10)
C4—H4A	0.9900	C33—H33A	0.9900
C4—H4B	0.9900	C33—H33B	0.9900
C5—C22	1.519 (10)	C34—C53	1.531 (10)
C5—C24	1.548 (10)	C34—C51	1.539 (10)
C5—C6	1.570 (9)	C34—C35	1.580 (9)
C6—C7	1.527 (10)	C35—C36	1.523 (9)
C6—C19	1.572 (10)	C35—C48	1.585 (9)
C6—H6	1.0000	C35—H35	1.0000
C7—C8	1.537 (9)	C36—C37	1.541 (9)
C7—H7A	0.9900	C36—H36A	0.9900

C7—H7B	0.9900	C36—H36B	0.9900
C8—C9	1.535 (10)	C37—C38	1.523 (10)
C8—H8A	0.9900	C37—H37A	0.9900
C8—H8B	0.9900	C37—H37B	0.9900
C9—C18	1.563 (10)	C38—C47	1.570 (9)
C9—C10	1.568 (9)	C38—C39	1.587 (9)
C9—H9	1.0000	C38—H38	1.0000
C10—C25	1.539 (9)	C39—C54	1.538 (10)
C10—C11	1.543 (10)	C39—C40	1.547 (10)
C10—C15	1.562 (10)	C39—C44	1.558 (10)
C11—C12	1.526 (9)	C40—C41	1.537 (9)
C11—H11A	0.9900	C40—H40A	0.9900
C11—H11B	0.9900	C40—H40B	0.9900
C12—C13	1.523 (10)	C41—C42	1.542 (12)
C12—H12A	0.9900	C41—H41A	0.9900
C12—H12B	0.9900	C41—H41B	0.9900
C13—C14	1.532 (10)	C42—C43	1.516 (10)
C13—H13A	0.9900	C42—H42A	0.9900
C13—H13B	0.9900	C42—H42B	0.9900
C14—C27	1.537 (10)	C43—C56	1.535 (10)
C14—C26	1.547 (10)	C43—C55	1.541 (10)
C14—C15	1.565 (9)	C43—C44	1.567 (9)
C15—C16	1.527 (10)	C44—C45	1.529 (10)
C15—H15	1.0000	C44—H44	1.0000
C16—C17	1.531 (9)	C45—C46	1.539 (9)
C16—H16A	0.9900	C45—H45A	0.9900
C16—H16B	0.9900	C45—H45B	0.9900
C17—C18	1.549 (10)	C46—C47	1.558 (9)
C17—H17A	0.9900	C46—H46A	0.9900
C17—H17B	0.9900	C46—H46B	0.9900
C18—C28	1.526 (10)	C47—C57	1.556 (10)
C18—C19	1.615 (9)	C47—C48	1.608 (9)
C19—C29	1.528 (10)	C48—C58	1.529 (10)
C19—C20	1.544 (10)	C48—C49	1.545 (10)
C20—C21	1.551 (9)	C49—C50	1.527 (9)
C20—H20A	0.9900	C49—H49A	0.9900
C20—H20B	0.9900	C49—H49B	0.9900
C21—C22	1.534 (10)	C50—C51	1.534 (10)
C21—H21A	0.9900	C50—H50A	0.9900
C21—H21B	0.9900	C50—H50B	0.9900
C22—H22	1.0000	C51—H51	1.0000
C23—H23A	0.9800	C52—H52A	0.9800
C23—H23B	0.9800	C52—H52B	0.9800
C23—H23C	0.9800	C52—H52C	0.9800
C24—H24A	0.9800	C53—H53A	0.9800
C24—H24B	0.9800	C53—H53B	0.9800
C24—H24C	0.9800	C53—H53C	0.9800
C25—H25A	0.9800	C54—H54A	0.9800

C25—H25B	0.9800	C54—H54B	0.9800
C25—H25C	0.9800	C54—H54C	0.9800
C26—H26A	0.9800	C55—H55A	0.9800
C26—H26B	0.9800	C55—H55B	0.9800
C26—H26C	0.9800	C55—H55C	0.9800
C27—H27A	0.9800	C56—H56A	0.9800
C27—H27B	0.9800	C56—H56B	0.9800
C27—H27C	0.9800	C56—H56C	0.9800
C28—H28A	0.9800	C57—H57A	0.9800
C28—H28B	0.9800	C57—H57B	0.9800
C28—H28C	0.9800	C57—H57C	0.9800
C29—H29A	0.9800	C58—H58A	0.9800
C29—H29B	0.9800	C58—H58B	0.9800
C29—H29C	0.9800	C58—H58C	0.9800

O1—C1—C2	109.0 (6)	O3—C30—C31	110.3 (6)
O1—C1—C23	108.3 (6)	O3—C30—C52	109.7 (7)
C2—C1—C23	108.7 (6)	C31—C30—C52	107.4 (7)
O1—C1—C22	106.1 (6)	O3—C30—C51	104.9 (6)
C2—C1—C22	108.4 (6)	C31—C30—C51	110.7 (6)
C23—C1—C22	116.1 (6)	C52—C30—C51	113.8 (6)
C1—O1—H1	109.5	C30—O3—H3	109.5
O2—C2—C3	123.0 (7)	O4—C31—C32	122.2 (8)
O2—C2—C1	119.5 (8)	O4—C31—C30	117.9 (8)
C3—C2—C1	117.5 (7)	C32—C31—C30	119.8 (7)
C2—C3—C4	111.7 (7)	C31—C32—C33	112.6 (7)
C2—C3—H3A	109.3	C31—C32—H32A	109.1
C4—C3—H3A	109.3	C33—C32—H32A	109.1
C2—C3—H3B	109.3	C31—C32—H32B	109.1
C4—C3—H3B	109.3	C33—C32—H32B	109.1
H3A—C3—H3B	107.9	H32A—C32—H32B	107.8
C3—C4—C5	113.3 (6)	C32—C33—C34	112.6 (6)
C3—C4—H4A	108.9	C32—C33—H33A	109.1
C5—C4—H4A	108.9	C34—C33—H33A	109.1
C3—C4—H4B	108.9	C32—C33—H33B	109.1
C5—C4—H4B	108.9	C34—C33—H33B	109.1
H4A—C4—H4B	107.7	H33A—C33—H33B	107.8
C22—C5—C24	114.5 (6)	C53—C34—C51	114.8 (6)
C22—C5—C4	107.7 (6)	C53—C34—C33	108.1 (6)
C24—C5—C4	106.3 (6)	C51—C34—C33	108.5 (6)
C22—C5—C6	106.9 (6)	C53—C34—C35	112.6 (6)
C24—C5—C6	113.0 (6)	C51—C34—C35	105.7 (6)
C4—C5—C6	108.2 (6)	C33—C34—C35	106.8 (6)
C7—C6—C5	114.3 (6)	C36—C35—C34	113.9 (6)
C7—C6—C19	109.1 (6)	C36—C35—C48	109.5 (6)
C5—C6—C19	116.4 (6)	C34—C35—C48	116.1 (6)
C7—C6—H6	105.3	C36—C35—H35	105.4
C5—C6—H6	105.3	C34—C35—H35	105.4

C19—C6—H6	105.3	C48—C35—H35	105.4
C6—C7—C8	112.9 (6)	C35—C36—C37	113.0 (6)
C6—C7—H7A	109.0	C35—C36—H36A	109.0
C8—C7—H7A	109.0	C37—C36—H36A	109.0
C6—C7—H7B	109.0	C35—C36—H36B	109.0
C8—C7—H7B	109.0	C37—C36—H36B	109.0
H7A—C7—H7B	107.8	H36A—C36—H36B	107.8
C9—C8—C7	112.5 (6)	C38—C37—C36	112.9 (6)
C9—C8—H8A	109.1	C38—C37—H37A	109.0
C7—C8—H8A	109.1	C36—C37—H37A	109.0
C9—C8—H8B	109.1	C38—C37—H37B	109.0
C7—C8—H8B	109.1	C36—C37—H37B	109.0
H8A—C8—H8B	107.8	H37A—C37—H37B	107.8
C8—C9—C18	109.2 (6)	C37—C38—C47	110.4 (6)
C8—C9—C10	113.8 (6)	C37—C38—C39	114.6 (6)
C18—C9—C10	117.0 (6)	C47—C38—C39	115.8 (6)
C8—C9—H9	105.2	C37—C38—H38	104.9
C18—C9—H9	105.2	C47—C38—H38	104.9
C10—C9—H9	105.2	C39—C38—H38	104.9
C25—C10—C11	108.0 (6)	C54—C39—C40	108.1 (6)
C25—C10—C15	113.4 (6)	C54—C39—C44	114.0 (6)
C11—C10—C15	107.0 (6)	C40—C39—C44	108.1 (6)
C25—C10—C9	112.5 (6)	C54—C39—C38	111.5 (6)
C11—C10—C9	108.6 (6)	C40—C39—C38	108.0 (6)
C15—C10—C9	107.0 (5)	C44—C39—C38	107.0 (6)
C12—C11—C10	113.7 (6)	C41—C40—C39	113.1 (6)
C12—C11—H11A	108.8	C41—C40—H40A	109.0
C10—C11—H11A	108.8	C39—C40—H40A	109.0
C12—C11—H11B	108.8	C41—C40—H40B	109.0
C10—C11—H11B	108.8	C39—C40—H40B	109.0
H11A—C11—H11B	107.7	H40A—C40—H40B	107.8
C13—C12—C11	111.4 (6)	C40—C41—C42	110.1 (7)
C13—C12—H12A	109.4	C40—C41—H41A	109.6
C11—C12—H12A	109.4	C42—C41—H41A	109.6
C13—C12—H12B	109.4	C40—C41—H41B	109.6
C11—C12—H12B	109.4	C42—C41—H41B	109.6
H12A—C12—H12B	108.0	H41A—C41—H41B	108.2
C12—C13—C14	114.4 (6)	C43—C42—C41	113.7 (7)
C12—C13—H13A	108.7	C43—C42—H42A	108.8
C14—C13—H13A	108.7	C41—C42—H42A	108.8
C12—C13—H13B	108.7	C43—C42—H42B	108.8
C14—C13—H13B	108.7	C41—C42—H42B	108.8
H13A—C13—H13B	107.6	H42A—C42—H42B	107.7
C13—C14—C27	106.7 (6)	C42—C43—C56	110.8 (6)
C13—C14—C26	111.1 (6)	C42—C43—C55	106.2 (7)
C27—C14—C26	107.6 (6)	C56—C43—C55	106.5 (6)
C13—C14—C15	108.6 (6)	C42—C43—C44	109.3 (6)
C27—C14—C15	108.3 (6)	C56—C43—C44	115.4 (6)

C26—C14—C15	114.1 (6)	C55—C43—C44	108.2 (6)
C16—C15—C10	110.8 (6)	C45—C44—C39	111.4 (6)
C16—C15—C14	114.2 (6)	C45—C44—C43	114.4 (6)
C10—C15—C14	116.4 (6)	C39—C44—C43	115.3 (6)
C16—C15—H15	104.7	C45—C44—H44	104.8
C10—C15—H15	104.7	C39—C44—H44	104.8
C14—C15—H15	104.7	C43—C44—H44	104.8
C15—C16—C17	110.7 (6)	C44—C45—C46	110.2 (6)
C15—C16—H16A	109.5	C44—C45—H45A	109.6
C17—C16—H16A	109.5	C46—C45—H45A	109.6
C15—C16—H16B	109.5	C44—C45—H45B	109.6
C17—C16—H16B	109.5	C46—C45—H45B	109.6
H16A—C16—H16B	108.1	H45A—C45—H45B	108.1
C16—C17—C18	114.3 (6)	C45—C46—C47	113.5 (6)
C16—C17—H17A	108.7	C45—C46—H46A	108.9
C18—C17—H17A	108.7	C47—C46—H46A	108.9
C16—C17—H17B	108.7	C45—C46—H46B	108.9
C18—C17—H17B	108.7	C47—C46—H46B	108.9
H17A—C17—H17B	107.6	H46A—C46—H46B	107.7
C28—C18—C17	107.3 (6)	C57—C47—C46	106.2 (6)
C28—C18—C9	112.1 (6)	C57—C47—C38	111.5 (6)
C17—C18—C9	108.0 (6)	C46—C47—C38	109.6 (6)
C28—C18—C19	111.2 (6)	C57—C47—C48	110.7 (5)
C17—C18—C19	110.0 (5)	C46—C47—C48	109.6 (6)
C9—C18—C19	108.2 (5)	C38—C47—C48	109.2 (5)
C29—C19—C20	106.5 (6)	C58—C48—C49	107.3 (6)
C29—C19—C6	111.6 (6)	C58—C48—C35	111.3 (6)
C20—C19—C6	108.9 (6)	C49—C48—C35	109.6 (5)
C29—C19—C18	112.0 (5)	C58—C48—C47	111.0 (5)
C20—C19—C18	110.1 (6)	C49—C48—C47	111.1 (6)
C6—C19—C18	107.7 (5)	C35—C48—C47	106.4 (6)
C19—C20—C21	113.2 (6)	C50—C49—C48	114.1 (6)
C19—C20—H20A	108.9	C50—C49—H49A	108.7
C21—C20—H20A	108.9	C48—C49—H49A	108.7
C19—C20—H20B	108.9	C50—C49—H49B	108.7
C21—C20—H20B	108.9	C48—C49—H49B	108.7
H20A—C20—H20B	107.7	H49A—C49—H49B	107.6
C22—C21—C20	109.7 (6)	C49—C50—C51	109.5 (6)
C22—C21—H21A	109.7	C49—C50—H50A	109.8
C20—C21—H21A	109.7	C51—C50—H50A	109.8
C22—C21—H21B	109.7	C49—C50—H50B	109.8
C20—C21—H21B	109.7	C51—C50—H50B	109.8
H21A—C21—H21B	108.2	H50A—C50—H50B	108.2
C5—C22—C21	111.5 (6)	C50—C51—C34	112.0 (6)
C5—C22—C1	117.8 (6)	C50—C51—C30	112.8 (6)
C21—C22—C1	111.7 (6)	C34—C51—C30	116.5 (6)
C5—C22—H22	104.9	C50—C51—H51	104.7
C21—C22—H22	104.9	C34—C51—H51	104.7

C1—C22—H22	104.9	C30—C51—H51	104.7
C1—C23—H23A	109.5	C30—C52—H52A	109.5
C1—C23—H23B	109.5	C30—C52—H52B	109.5
H23A—C23—H23B	109.5	H52A—C52—H52B	109.5
C1—C23—H23C	109.5	C30—C52—H52C	109.5
H23A—C23—H23C	109.5	H52A—C52—H52C	109.5
H23B—C23—H23C	109.5	H52B—C52—H52C	109.5
C5—C24—H24A	109.5	C34—C53—H53A	109.5
C5—C24—H24B	109.5	C34—C53—H53B	109.5
H24A—C24—H24B	109.5	H53A—C53—H53B	109.5
C5—C24—H24C	109.5	C34—C53—H53C	109.5
H24A—C24—H24C	109.5	H53A—C53—H53C	109.5
H24B—C24—H24C	109.5	H53B—C53—H53C	109.5
C10—C25—H25A	109.5	C39—C54—H54A	109.5
C10—C25—H25B	109.5	C39—C54—H54B	109.5
H25A—C25—H25B	109.5	H54A—C54—H54B	109.5
C10—C25—H25C	109.5	C39—C54—H54C	109.5
H25A—C25—H25C	109.5	H54A—C54—H54C	109.5
H25B—C25—H25C	109.5	H54B—C54—H54C	109.5
C14—C26—H26A	109.5	C43—C55—H55A	109.5
C14—C26—H26B	109.5	C43—C55—H55B	109.5
H26A—C26—H26B	109.5	H55A—C55—H55B	109.5
C14—C26—H26C	109.5	C43—C55—H55C	109.5
H26A—C26—H26C	109.5	H55A—C55—H55C	109.5
H26B—C26—H26C	109.5	H55B—C55—H55C	109.5
C14—C27—H27A	109.5	C43—C56—H56A	109.5
C14—C27—H27B	109.5	C43—C56—H56B	109.5
H27A—C27—H27B	109.5	H56A—C56—H56B	109.5
C14—C27—H27C	109.5	C43—C56—H56C	109.5
H27A—C27—H27C	109.5	H56A—C56—H56C	109.5
H27B—C27—H27C	109.5	H56B—C56—H56C	109.5
C18—C28—H28A	109.5	C47—C57—H57A	109.5
C18—C28—H28B	109.5	C47—C57—H57B	109.5
H28A—C28—H28B	109.5	H57A—C57—H57B	109.5
C18—C28—H28C	109.5	C47—C57—H57C	109.5
H28A—C28—H28C	109.5	H57A—C57—H57C	109.5
H28B—C28—H28C	109.5	H57B—C57—H57C	109.5
C19—C29—H29A	109.5	C48—C58—H58A	109.5
C19—C29—H29B	109.5	C48—C58—H58B	109.5
H29A—C29—H29B	109.5	H58A—C58—H58B	109.5
C19—C29—H29C	109.5	C48—C58—H58C	109.5
H29A—C29—H29C	109.5	H58A—C58—H58C	109.5
H29B—C29—H29C	109.5	H58B—C58—H58C	109.5

O1—C1—C2—O2	17.6 (9)	O3—C30—C31—O4	26.7 (10)
C23—C1—C2—O2	−100.3 (8)	C52—C30—C31—O4	−92.9 (8)
C22—C1—C2—O2	132.7 (7)	C51—C30—C31—O4	142.3 (7)
O1—C1—C2—C3	−161.4 (6)	O3—C30—C31—C32	−155.2 (7)

C23—C1—C2—C3	80.7 (8)	C52—C30—C31—C32	85.2 (8)
C22—C1—C2—C3	−46.2 (9)	C51—C30—C31—C32	−39.6 (10)
O2—C2—C3—C4	−128.5 (8)	O4—C31—C32—C33	−137.7 (8)
C1—C2—C3—C4	50.4 (9)	C30—C31—C32—C33	44.3 (10)
C2—C3—C4—C5	−53.1 (9)	C31—C32—C33—C34	−51.2 (10)
C3—C4—C5—C22	53.5 (9)	C32—C33—C34—C53	−69.9 (8)
C3—C4—C5—C24	−69.6 (8)	C32—C33—C34—C51	55.1 (8)
C3—C4—C5—C6	168.8 (7)	C32—C33—C34—C35	168.6 (6)
C22—C5—C6—C7	177.2 (6)	C53—C34—C35—C36	−56.1 (9)
C24—C5—C6—C7	−56.0 (9)	C51—C34—C35—C36	177.9 (6)
C4—C5—C6—C7	61.4 (8)	C33—C34—C35—C36	62.5 (8)
C22—C5—C6—C19	−54.2 (8)	C53—C34—C35—C48	72.5 (8)
C24—C5—C6—C19	72.7 (8)	C51—C34—C35—C48	−53.5 (8)
C4—C5—C6—C19	−169.9 (6)	C33—C34—C35—C48	−168.9 (6)
C5—C6—C7—C8	−170.9 (6)	C34—C35—C36—C37	−170.6 (6)
C19—C6—C7—C8	56.8 (8)	C48—C35—C36—C37	57.5 (8)
C6—C7—C8—C9	−55.0 (9)	C35—C36—C37—C38	−53.4 (9)
C7—C8—C9—C18	56.1 (8)	C36—C37—C38—C47	53.2 (8)
C7—C8—C9—C10	−171.1 (6)	C36—C37—C38—C39	−173.9 (6)
C8—C9—C10—C25	−57.9 (8)	C37—C38—C39—C54	−58.3 (9)
C18—C9—C10—C25	71.1 (8)	C47—C38—C39—C54	72.0 (8)
C8—C9—C10—C11	61.7 (8)	C37—C38—C39—C40	60.3 (8)
C18—C9—C10—C11	−169.3 (6)	C47—C38—C39—C40	−169.4 (6)
C8—C9—C10—C15	176.9 (6)	C37—C38—C39—C44	176.5 (6)
C18—C9—C10—C15	−54.1 (8)	C47—C38—C39—C44	−53.2 (8)
C25—C10—C11—C12	−67.9 (8)	C54—C39—C40—C41	−69.2 (9)
C15—C10—C11—C12	54.5 (8)	C44—C39—C40—C41	54.6 (9)
C9—C10—C11—C12	169.7 (6)	C38—C39—C40—C41	170.1 (7)
C10—C11—C12—C13	−56.7 (8)	C39—C40—C41—C42	−57.2 (9)
C11—C12—C13—C14	54.3 (8)	C40—C41—C42—C43	56.4 (9)
C12—C13—C14—C27	−167.0 (6)	C41—C42—C43—C56	75.4 (8)
C12—C13—C14—C26	75.9 (8)	C41—C42—C43—C55	−169.4 (6)
C12—C13—C14—C15	−50.4 (8)	C41—C42—C43—C44	−52.9 (9)
C25—C10—C15—C16	−67.1 (7)	C54—C39—C44—C45	−64.9 (8)
C11—C10—C15—C16	173.9 (6)	C40—C39—C44—C45	174.9 (6)
C9—C10—C15—C16	57.6 (7)	C38—C39—C44—C45	58.8 (8)
C25—C10—C15—C14	65.6 (8)	C54—C39—C44—C43	67.6 (8)
C11—C10—C15—C14	−53.4 (8)	C40—C39—C44—C43	−52.6 (8)
C9—C10—C15—C14	−169.7 (6)	C38—C39—C44—C43	−168.7 (6)
C13—C14—C15—C16	−177.2 (6)	C42—C43—C44—C45	−176.7 (7)
C27—C14—C15—C16	−61.6 (8)	C56—C43—C44—C45	57.6 (9)
C26—C14—C15—C16	58.2 (9)	C55—C43—C44—C45	−61.5 (9)
C13—C14—C15—C10	51.7 (8)	C42—C43—C44—C39	52.2 (9)
C27—C14—C15—C10	167.3 (6)	C56—C43—C44—C39	−73.5 (9)
C26—C14—C15—C10	−72.9 (9)	C55—C43—C44—C39	167.4 (6)
C10—C15—C16—C17	−61.2 (8)	C39—C44—C45—C46	−62.6 (8)
C14—C15—C16—C17	165.0 (6)	C43—C44—C45—C46	164.4 (7)
C15—C16—C17—C18	57.7 (9)	C44—C45—C46—C47	57.5 (9)

C16—C17—C18—C28	71.4 (8)	C45—C46—C47—C57	71.0 (8)
C16—C17—C18—C9	−49.6 (8)	C45—C46—C47—C38	−49.6 (9)
C16—C17—C18—C19	−167.5 (6)	C45—C46—C47—C48	−169.4 (6)
C8—C9—C18—C28	62.8 (7)	C37—C38—C47—C57	63.8 (7)
C10—C9—C18—C28	−68.3 (8)	C39—C38—C47—C57	−68.5 (8)
C8—C9—C18—C17	−179.2 (5)	C37—C38—C47—C46	−178.8 (6)
C10—C9—C18—C17	49.6 (8)	C39—C38—C47—C46	48.8 (8)
C8—C9—C18—C19	−60.2 (7)	C37—C38—C47—C48	−58.8 (8)
C10—C9—C18—C19	168.6 (6)	C39—C38—C47—C48	168.9 (6)
C7—C6—C19—C29	63.0 (7)	C36—C35—C48—C58	59.8 (8)
C5—C6—C19—C29	−68.2 (8)	C34—C35—C48—C58	−70.8 (8)
C7—C6—C19—C20	−179.8 (6)	C36—C35—C48—C49	178.4 (6)
C5—C6—C19—C20	49.0 (8)	C34—C35—C48—C49	47.7 (8)
C7—C6—C19—C18	−60.4 (7)	C36—C35—C48—C47	−61.3 (7)
C5—C6—C19—C18	168.4 (6)	C34—C35—C48—C47	168.0 (6)
C28—C18—C19—C29	176.3 (6)	C57—C47—C48—C58	177.9 (6)
C17—C18—C19—C29	57.7 (8)	C46—C47—C48—C58	61.0 (8)
C9—C18—C19—C29	−60.1 (7)	C38—C47—C48—C58	−59.0 (8)
C28—C18—C19—C20	58.1 (8)	C57—C47—C48—C49	58.5 (8)
C17—C18—C19—C20	−60.6 (7)	C46—C47—C48—C49	−58.3 (8)
C9—C18—C19—C20	−178.3 (6)	C38—C47—C48—C49	−178.4 (6)
C28—C18—C19—C6	−60.5 (7)	C57—C47—C48—C35	−60.8 (7)
C17—C18—C19—C6	−179.2 (6)	C46—C47—C48—C35	−177.7 (6)
C9—C18—C19—C6	63.1 (7)	C38—C47—C48—C35	62.3 (7)
C29—C19—C20—C21	71.3 (8)	C58—C48—C49—C50	73.2 (8)
C6—C19—C20—C21	−49.2 (8)	C35—C48—C49—C50	−47.9 (9)
C18—C19—C20—C21	−167.0 (6)	C47—C48—C49—C50	−165.3 (6)
C19—C20—C21—C22	57.3 (8)	C48—C49—C50—C51	56.6 (9)
C24—C5—C22—C21	−66.2 (8)	C49—C50—C51—C34	−64.2 (8)
C4—C5—C22—C21	175.9 (6)	C49—C50—C51—C30	161.9 (6)
C6—C5—C22—C21	59.7 (8)	C53—C34—C51—C50	−64.0 (8)
C24—C5—C22—C1	64.8 (8)	C33—C34—C51—C50	175.0 (6)
C4—C5—C22—C1	−53.1 (8)	C35—C34—C51—C50	60.7 (8)
C6—C5—C22—C1	−169.2 (6)	C53—C34—C51—C30	68.0 (8)
C20—C21—C22—C5	−63.2 (8)	C33—C34—C51—C30	−53.0 (8)
C20—C21—C22—C1	162.7 (6)	C35—C34—C51—C30	−167.3 (6)
O1—C1—C22—C5	166.1 (6)	O3—C30—C51—C50	−64.9 (8)
C2—C1—C22—C5	49.0 (9)	C31—C30—C51—C50	176.1 (6)
C23—C1—C22—C5	−73.5 (9)	C52—C30—C51—C50	55.0 (9)
O1—C1—C22—C21	−63.0 (8)	O3—C30—C51—C34	163.5 (6)
C2—C1—C22—C21	180.0 (7)	C31—C30—C51—C34	44.5 (9)
C23—C1—C22—C21	57.4 (9)	C52—C30—C51—C34	−76.6 (9)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O4	0.84	2.19	2.978 (8)	156
O3—H3···O5	0.84	2.06	2.896 (9)	176