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(2*S*,3*S*)-2-Azaniumyl-4-[(1*S*,4a*S*,4b*S*,6*S*,7*S*,8a*S*,10a*S*)-6,7-dihydroxy-2,4b,8,8,10a-pentamethyl-1,4,4a,4b,5,6,7,8,8a,9,10,10a-dodecahydrophenanthren-1-yl]-3-methoxybutanoate–methanol–water (1/1/1)

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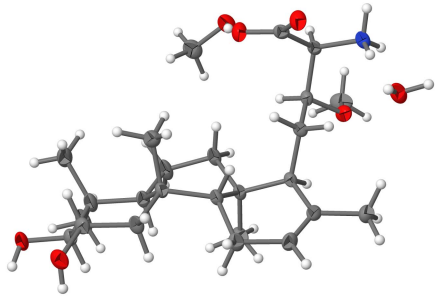
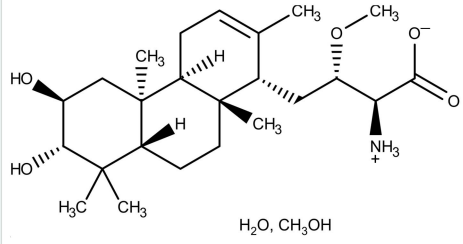
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, which crystallized as a methanol and water solvate, $C_{24}H_{41}NO_5\cdot CH_4O\cdot H_2O$, was obtained by heterologous expression of the brasilicardin gene cluster in the bacterium *Amycolatopsis japonicum*. In the crystal, the components are linked by numerous hydrogen bonds, generating a three-dimensional network.

3D view



Chemical scheme



Structure description

The title compound (Fig. 1), representing the aglycone of the natural products brasilicardin A and brasilicardin C, was obtained by heterologous expression of the brasilicardin gene cluster (Buchmann *et al.* 2016) in *Amycolatopsis japonicum* (Schwarz *et al.* 2018*a*,*b*). As a result of the *anti–syn–anti* configured *B* ring within the perhydrophenanthrene system, this tricyclic system is in an unusual chair–boat–chair conformation. For crystal structures of compounds having the same perhydrophenanthrene core, see Shigemori *et al.* (1998) and Komatsu *et al.* (2004).

The crystal packing is consolidated by a three-dimensional network of numerous hydrogen bonds (Table 1, Fig. 2).

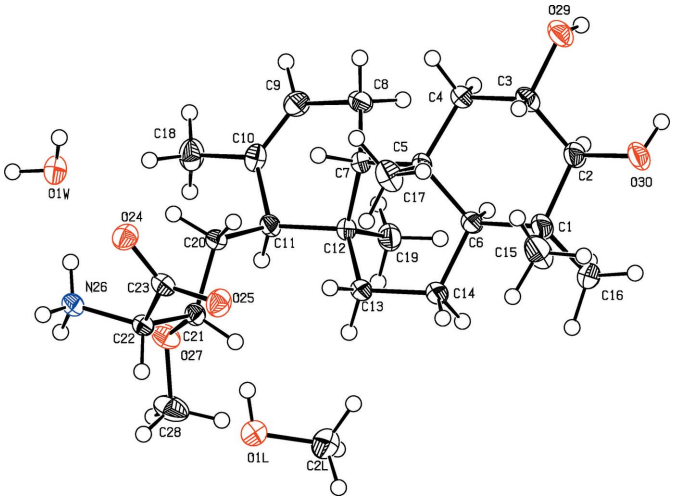


Figure 1
Molecular structure of the title compound with the atom labelling and displacement ellipsoids drawn at the 50% probability level.

Synthesis and crystallization

The title compound $C_{24}H_{41}NO_5$ was isolated from a fermentation broth of *Amycolatopsis japonicum::bcaAB01*, which was cultivated under brasilicardin production conditions for 3 d (Schwarz *et al.* 2018*a*,*b*). The extract was purified by flash chromatography followed by preparative HPLC to yield the product $C_{24}H_{41}NO_5$ as a white solid. The solid was dissolved in a minimum of methanol and crystals suitable for X-ray determination were subsequently obtained by slow evaporation of the solvent at 298 K.

^{1}H NMR (400 MHz, CD_3OD) δ 5.30 (*br s*, 1H), 3.95 (*d*, *J* = 3.5 Hz, 1H), 3.75 (*dd*, *J* = 11.2, 2.9 Hz, 1H), 3.57 (*ddd*, *J* = 11.2, 9.7, 4.2 Hz, 1H), 3.45 (*s*, 3H), 2.85 (*d*, *J* = 9.5 Hz, 1H), 1.94–1.78 (*m*, 3H), 1.74–1.66 (*m*, 2H), 1.65 (*s*, 3H), 1.64–1.53 (*m*, 4H), 1.36–1.24 (*m*, 4H), 1.10 (*s*, 3H), 1.02 (*s*, 3H), 0.96 (*s*, 3H), 0.89 (*s*, 3H). ^{13}C NMR (101 MHz, CD_3OD) δ 171.5, 138.9, 123.3, 84.6, 81.2, 70.2, 57.9, 56.2, 52.5, 47.2, 45.0, 44.6, 41.0, 38.6, 37.6, 31.7, 31.2, 29.4, 29.1, 27.0, 23.1, 22.7, 18.8, 17.4. MS (ESI) calculated for $C_{24}H_{41}NO_5$ $(M - H)^-$ 422.3, found 422.4.

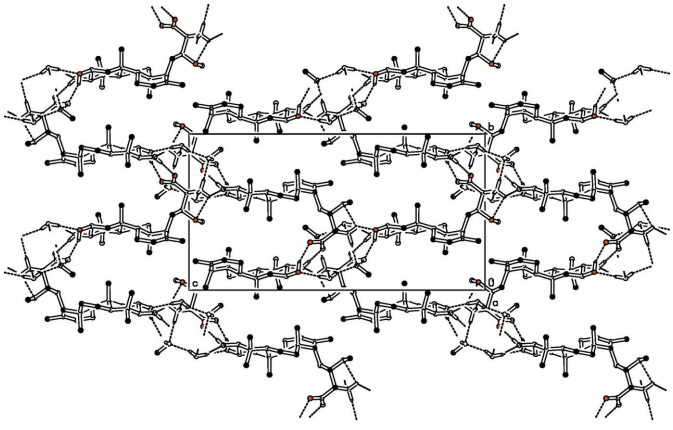


Figure 2
Part of the crystal packing. View along the *a* axis. Hydrogen bonds are indicated by dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*L*—H1*L*···O25	0.86 (4)	1.81 (4)	2.662 (3)	171 (4)
O1*W*—H1*W*···O29^{i}	0.87 (4)	1.92 (4)	2.767 (3)	162 (4)
O1*W*—H2*W*···O1*L*^{ii}	0.83 (4)	2.15 (4)	2.948 (3)	162 (4)
C20—H20*B*···O1*W*	0.99 (3)	2.47 (3)	3.423 (3)	162 (2)
C22—H22···O24^{iii}	0.93 (3)	2.54 (3)	3.385 (3)	151 (3)
N26—H26*A*···O30^{iv}	0.92 (4)	2.24 (4)	2.846 (3)	123 (3)
N26—H26*B*···O1*L*^{v}	0.92 (4)	1.95 (4)	2.869 (3)	172 (4)
N26—H26*C*···O1*W*	0.86 (4)	1.95 (4)	2.798 (3)	169 (3)
C28—H28*A*···O30^{iv}	0.96 (4)	2.51 (4)	3.346 (4)	144 (3)
O29—H29···O25^{vi}	0.84 (4)	1.97 (4)	2.769 (3)	157 (4)
O30—H30···O24^{vi}	0.84 (4)	1.85 (4)	2.680 (3)	171 (4)

Symmetry codes: (i) $-x+\frac{3}{2}, -y+1, z-\frac{1}{2}$; (ii) $x+1, y, z$; (iii) $x-\frac{1}{2}, -y+\frac{3}{2}, -z$; (iv) $-x+\frac{1}{2}, -y+1, z-\frac{1}{2}$; (v) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$; (vi) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{41}NO_5{\cdot}CH_4O{\cdot}H_2O$
M_r	473.63
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	193
a, *b*, *c* (Å)	7.9093 (2), 13.3712 (4), 25.3669 (7)
V (Å^3)	2682.72 (13)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.45 × 0.09 × 0.08
Data collection	
Diffractometer	Stoe IPDS 2T
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17021, 6656, 5482
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.049, 0.098, 1.07
No. of reflections	6656
No. of parameters	465
H-atom treatment	Only H-atom coordinates refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.19
Absolute structure	Flack *x* determined using 1941 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter	−0.6 (7)

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 2011), *SIR2004* (Burla *et al.*, 2005) and *SHELXL2014* (Sheldrick, 2015).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The absolute structure was indeterminate based on the present refinement. The title compound (brasilicardin aglycone) was produced by a fermentation process and we assumed that the stereochemistry of the the title compound is the same as (1) the stereochemistry of the reported natural products Brasilicardin A and Brasilicardin C (the latter one was also obtained during

our fermentation process) as well as (2) the stereochemistry of the title compound reported in the proposed biosynthetic pathway scheme of Brasilicardins A and C (Hayashi *et al.*, 2008). This defines the configurations of the stereogenic centres as C2 *S*, C3 *S*, C5 *S*, C6 *S*, C7 *R*, C11 *S*, C12 *S*, C21, *S* and C22 *S*.

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x181194 [https://doi.org/10.1107/S241431461801194X]

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(2*S*,3*S*)-2-Azaniumyl-4-[(1*S*,4a*S*,4b*S*,6*S*,7*S*,8a*S*,10a*S*)-6,7-dihydroxy-2,4b,8,8,10a-pentamethyl-1,4,4a,4b,5,6,7,8,8a,9,10,10a-dodecahydrophenanthren-1-yl]-3-methoxybutanoate–methanol–water (1/1/1)

Crystal data

$C_{24}H_{41}NO_5 \cdot CH_4O \cdot H_2O$
M_r = 473.63
Orthorhombic, $P2_12_12_1$
a = 7.9093 (2) Å
b = 13.3712 (4) Å
c = 25.3669 (7) Å
V = 2682.72 (13) Å^3
Z = 4
$F(000)$ = 1040
D_x = 1.173 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 15328 reflections
θ = 1.7–28.4°
μ = 0.08 mm^{-1}
T = 193 K
Coloumn, colourless
0.45 × 0.09 × 0.08 mm

Data collection

Stoe IPDS 2T diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
17021 measured reflections
6656 independent reflections
5482 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 28.3°, θ_{min} = 1.7°
h = −10→9
k = −17→17
l = −33→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.098
S = 1.07
6656 reflections
465 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0216P)^2 + 1.5011P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Absolute structure: Flack x determined using 1941 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter: −0.6 (7)

Special details

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. All the hydrogen atoms were localized in difference maps and their positions were refined with isotropic displacement parameters.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1L	−0.0039 (3)	0.65612 (17)	0.06774 (9)	0.0321 (5)
H1L	0.098 (5)	0.664 (3)	0.0782 (15)	0.040 (10)*
C2L	−0.0906 (5)	0.5995 (3)	0.10662 (15)	0.0377 (8)
H2L	−0.209 (6)	0.625 (3)	0.1094 (16)	0.062 (8)*
H3L	−0.031 (6)	0.603 (3)	0.1424 (17)	0.062 (8)*
H4L	−0.099 (5)	0.526 (3)	0.0962 (17)	0.062 (8)*
O1W	0.8169 (3)	0.57637 (18)	−0.02510 (10)	0.0316 (5)
H1W	0.856 (5)	0.586 (3)	−0.0569 (16)	0.046 (8)*
H2W	0.879 (5)	0.606 (3)	−0.0042 (16)	0.046 (8)*
C1	0.2183 (4)	0.3791 (3)	0.29186 (11)	0.0295 (7)
C2	0.3519 (4)	0.3486 (2)	0.33292 (11)	0.0250 (6)
H2	0.383 (4)	0.277 (2)	0.3247 (12)	0.019 (8)*
C3	0.5130 (4)	0.4103 (2)	0.32866 (11)	0.0245 (6)
H3	0.486 (4)	0.481 (2)	0.3363 (12)	0.021 (8)*
C4	0.5913 (3)	0.3976 (2)	0.27431 (11)	0.0234 (6)
H4A	0.621 (4)	0.326 (3)	0.2696 (13)	0.027 (6)*
H4B	0.701 (4)	0.436 (2)	0.2730 (12)	0.027 (6)*
C5	0.4738 (3)	0.4269 (2)	0.22846 (11)	0.0211 (6)
C6	0.3031 (3)	0.3733 (2)	0.23637 (11)	0.0237 (6)
H6	0.331 (4)	0.299 (2)	0.2338 (11)	0.015 (7)*
C7	0.5516 (3)	0.3947 (2)	0.17323 (10)	0.0194 (5)
H7	0.598 (4)	0.459 (2)	0.1579 (11)	0.015 (7)*
C8	0.7041 (4)	0.3244 (2)	0.17471 (12)	0.0258 (6)
H8A	0.797 (4)	0.353 (2)	0.1952 (13)	0.030 (6)*
H8B	0.678 (4)	0.261 (3)	0.1930 (13)	0.030 (6)*
C9	0.7706 (4)	0.3079 (2)	0.11968 (12)	0.0270 (6)
H9	0.883 (4)	0.280 (2)	0.1177 (13)	0.030 (9)*
C10	0.6879 (4)	0.3311 (2)	0.07569 (11)	0.0234 (6)
C11	0.5097 (3)	0.3730 (2)	0.07633 (10)	0.0194 (5)
H11	0.450 (4)	0.335 (2)	0.0491 (12)	0.020 (8)*
C12	0.4250 (3)	0.3558 (2)	0.13094 (10)	0.0199 (5)
C13	0.2593 (3)	0.4127 (2)	0.13744 (11)	0.0245 (6)
H13A	0.182 (4)	0.391 (2)	0.1089 (12)	0.023 (6)*
H13B	0.281 (4)	0.486 (2)	0.1316 (12)	0.023 (6)*
C14	0.1764 (4)	0.3940 (3)	0.19145 (12)	0.0313 (7)
H14A	0.099 (5)	0.337 (3)	0.1884 (15)	0.042 (7)*
H14B	0.101 (5)	0.452 (3)	0.2025 (15)	0.042 (7)*

C15	0.1417 (5)	0.4816 (3)	0.30652 (15)	0.0449 (10)
H15A	0.230 (6)	0.531 (3)	0.3128 (18)	0.069 (8)*
H15B	0.087 (6)	0.475 (3)	0.3390 (19)	0.069 (8)*
H15C	0.064 (6)	0.505 (3)	0.2776 (19)	0.069 (8)*
C16	0.0749 (4)	0.3022 (3)	0.29376 (14)	0.0408 (9)
H16A	−0.028 (5)	0.324 (3)	0.2697 (14)	0.044 (6)*
H16B	0.034 (5)	0.296 (3)	0.3297 (16)	0.044 (6)*
H16C	0.123 (5)	0.238 (3)	0.2831 (15)	0.044 (6)*
C17	0.4580 (5)	0.5423 (2)	0.22788 (14)	0.0324 (7)
H17A	0.571 (5)	0.570 (3)	0.2210 (15)	0.046 (6)*
H17B	0.426 (5)	0.571 (3)	0.2631 (16)	0.046 (6)*
H17C	0.375 (5)	0.565 (3)	0.2013 (15)	0.046 (6)*
C18	0.7657 (4)	0.3147 (3)	0.02232 (14)	0.0322 (7)
H18A	0.694 (5)	0.274 (3)	−0.0009 (15)	0.046 (6)*
H18B	0.871 (5)	0.278 (3)	0.0249 (15)	0.046 (6)*
H18C	0.784 (5)	0.377 (3)	0.0029 (14)	0.046 (6)*
C19	0.3867 (4)	0.2422 (2)	0.13407 (13)	0.0276 (6)
H19A	0.302 (5)	0.224 (3)	0.1063 (15)	0.047 (6)*
H19B	0.335 (5)	0.220 (3)	0.1681 (16)	0.047 (6)*
H19C	0.482 (5)	0.203 (3)	0.1262 (15)	0.047 (6)*
C20	0.5108 (3)	0.4819 (2)	0.05625 (11)	0.0192 (5)
H20A	0.522 (4)	0.529 (2)	0.0871 (12)	0.021 (5)*
H20B	0.611 (4)	0.495 (2)	0.0340 (12)	0.021 (5)*
C21	0.3581 (3)	0.5118 (2)	0.02327 (10)	0.0192 (5)
H21	0.256 (4)	0.503 (2)	0.0441 (12)	0.023*
C22	0.3638 (3)	0.6232 (2)	0.00644 (10)	0.0199 (5)
H22	0.257 (4)	0.642 (2)	−0.0047 (11)	0.021 (8)*
C23	0.4186 (3)	0.6903 (2)	0.05199 (11)	0.0217 (6)
O24	0.5567 (2)	0.73372 (15)	0.04793 (8)	0.0266 (5)
O25	0.3182 (3)	0.69380 (16)	0.09077 (8)	0.0277 (5)
N26	0.4811 (3)	0.6366 (2)	−0.03900 (9)	0.0228 (5)
H26A	0.441 (4)	0.599 (3)	−0.0668 (15)	0.035 (9)*
H26B	0.476 (5)	0.703 (3)	−0.0493 (15)	0.048 (11)*
H26C	0.583 (5)	0.622 (3)	−0.0309 (14)	0.033 (9)*
O27	0.3531 (3)	0.44976 (14)	−0.02207 (8)	0.0264 (5)
C28	0.1883 (5)	0.4378 (3)	−0.04375 (15)	0.0372 (8)
H28A	0.146 (5)	0.499 (3)	−0.0587 (15)	0.043 (6)*
H28B	0.114 (5)	0.412 (3)	−0.0142 (15)	0.043 (6)*
H28C	0.201 (5)	0.386 (3)	−0.0738 (15)	0.043 (6)*
O29	0.6326 (3)	0.38410 (18)	0.36899 (8)	0.0292 (5)
H29	0.644 (5)	0.322 (3)	0.3725 (17)	0.056 (13)*
O30	0.2805 (3)	0.35337 (18)	0.38417 (8)	0.0316 (5)
H30	0.342 (5)	0.319 (3)	0.4043 (16)	0.050 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1L	0.0246 (11)	0.0397 (12)	0.0319 (12)	−0.0017 (10)	−0.0002 (9)	0.0074 (10)

C2L	0.0330 (17)	0.040 (2)	0.040 (2)	−0.0047 (15)	0.0026 (15)	0.0076 (16)
O1W	0.0296 (11)	0.0384 (13)	0.0267 (12)	−0.0017 (10)	0.0056 (10)	0.0071 (10)
C1	0.0246 (14)	0.0452 (18)	0.0187 (14)	0.0086 (13)	0.0035 (11)	0.0082 (13)
C2	0.0249 (14)	0.0324 (15)	0.0178 (14)	0.0049 (13)	0.0031 (11)	0.0029 (12)
C3	0.0286 (14)	0.0285 (15)	0.0163 (13)	0.0032 (12)	−0.0034 (11)	0.0003 (11)
C4	0.0210 (13)	0.0315 (16)	0.0176 (14)	−0.0011 (12)	−0.0018 (11)	0.0027 (12)
C5	0.0213 (13)	0.0258 (13)	0.0163 (13)	0.0027 (11)	0.0028 (10)	0.0031 (11)
C6	0.0187 (12)	0.0346 (16)	0.0177 (14)	0.0045 (12)	0.0006 (10)	0.0045 (12)
C7	0.0182 (12)	0.0241 (13)	0.0158 (13)	−0.0006 (11)	0.0003 (10)	0.0022 (11)
C8	0.0209 (13)	0.0367 (17)	0.0198 (14)	0.0056 (13)	−0.0019 (11)	0.0030 (12)
C9	0.0216 (14)	0.0329 (15)	0.0265 (16)	0.0068 (12)	0.0043 (11)	−0.0007 (13)
C10	0.0263 (13)	0.0197 (13)	0.0240 (14)	−0.0014 (11)	0.0062 (12)	0.0008 (11)
C11	0.0216 (12)	0.0219 (13)	0.0146 (12)	−0.0006 (11)	−0.0012 (10)	0.0009 (10)
C12	0.0185 (12)	0.0249 (13)	0.0163 (13)	−0.0004 (11)	0.0017 (10)	0.0028 (11)
C13	0.0185 (13)	0.0378 (17)	0.0173 (14)	0.0009 (12)	−0.0006 (10)	0.0048 (12)
C14	0.0189 (14)	0.054 (2)	0.0208 (15)	0.0051 (15)	0.0014 (11)	0.0109 (14)
C15	0.044 (2)	0.063 (2)	0.0276 (18)	0.031 (2)	0.0105 (16)	0.0109 (18)
C16	0.0227 (15)	0.074 (3)	0.0263 (17)	−0.0019 (17)	0.0036 (13)	0.0157 (18)
C17	0.0434 (19)	0.0291 (16)	0.0247 (16)	0.0068 (14)	0.0003 (14)	0.0009 (13)
C18	0.0359 (17)	0.0325 (17)	0.0283 (17)	0.0065 (14)	0.0105 (14)	0.0021 (14)
C19	0.0317 (16)	0.0282 (15)	0.0229 (15)	−0.0065 (13)	−0.0009 (13)	0.0031 (12)
C20	0.0182 (12)	0.0218 (12)	0.0175 (13)	−0.0017 (10)	−0.0026 (10)	0.0015 (11)
C21	0.0205 (12)	0.0224 (13)	0.0148 (12)	−0.0017 (11)	−0.0001 (10)	−0.0005 (11)
C22	0.0183 (12)	0.0236 (13)	0.0178 (13)	0.0020 (11)	−0.0010 (10)	0.0025 (11)
C23	0.0242 (13)	0.0207 (13)	0.0203 (14)	0.0015 (11)	−0.0048 (11)	0.0016 (11)
O24	0.0257 (10)	0.0301 (10)	0.0240 (11)	−0.0067 (9)	0.0000 (8)	−0.0047 (8)
O25	0.0282 (10)	0.0318 (11)	0.0232 (11)	−0.0027 (9)	0.0044 (9)	−0.0040 (8)
N26	0.0232 (12)	0.0285 (13)	0.0167 (12)	−0.0027 (11)	−0.0029 (9)	0.0016 (10)
O27	0.0302 (10)	0.0275 (10)	0.0214 (10)	0.0017 (9)	−0.0068 (9)	−0.0045 (8)
C28	0.0405 (18)	0.0313 (17)	0.040 (2)	−0.0045 (15)	−0.0196 (16)	−0.0011 (15)
O29	0.0352 (12)	0.0338 (12)	0.0187 (10)	−0.0026 (10)	−0.0071 (9)	0.0021 (9)
O30	0.0310 (11)	0.0463 (13)	0.0174 (10)	0.0134 (10)	0.0049 (9)	0.0091 (10)

Geometric parameters (Å, º)

O1L—C2L	1.420 (4)	C13—C14	1.539 (4)
O1L—H1L	0.86 (4)	C13—H13A	0.99 (3)
C2L—H2L	1.00 (4)	C13—H13B	1.01 (3)
C2L—H3L	1.02 (4)	C14—H14A	0.99 (4)
C2L—H4L	1.02 (5)	C14—H14B	1.02 (4)
O1W—H1W	0.87 (4)	C15—H15A	0.97 (5)
O1W—H2W	0.83 (4)	C15—H15B	0.94 (5)
C1—C16	1.531 (5)	C15—H15C	1.00 (5)
C1—C2	1.539 (4)	C16—H16A	1.06 (4)
C1—C15	1.544 (5)	C16—H16B	0.97 (4)
C1—C6	1.561 (4)	C16—H16C	0.98 (4)
C2—O30	1.419 (3)	C17—H17A	0.99 (4)
C2—C3	1.522 (4)	C17—H17B	1.00 (4)

C2—H2	1.01 (3)	C17—H17C	0.99 (4)
C3—O29	1.436 (3)	C18—H18A	0.98 (4)
C3—C4	1.521 (4)	C18—H18B	0.97 (4)
C3—H3	0.99 (3)	C18—H18C	0.98 (4)
C4—C5	1.539 (4)	C19—H19A	1.00 (4)
C4—H4A	0.99 (3)	C19—H19B	1.00 (4)
C4—H4B	1.00 (3)	C19—H19C	0.94 (4)
C5—C6	1.542 (4)	C20—C21	1.523 (4)
C5—C17	1.549 (4)	C20—H20A	1.01 (3)
C5—C7	1.590 (4)	C20—H20B	0.99 (3)
C6—C14	1.542 (4)	C21—O27	1.419 (3)
C6—H6	1.02 (3)	C21—C22	1.550 (4)
C7—C8	1.529 (4)	C21—H21	0.97 (3)
C7—C12	1.557 (4)	C22—N26	1.490 (4)
C7—H7	1.02 (3)	C22—C23	1.525 (4)
C8—C9	1.508 (4)	C22—H22	0.93 (3)
C8—H8A	0.98 (3)	C23—O24	1.242 (3)
C8—H8B	0.98 (3)	C23—O25	1.265 (3)
C9—C10	1.330 (4)	N26—H26A	0.92 (4)
C9—H9	0.96 (3)	N26—H26B	0.92 (4)
C10—C18	1.503 (4)	N26—H26C	0.86 (4)
C10—C11	1.517 (4)	O27—C28	1.424 (4)
C11—C20	1.543 (4)	C28—H28A	0.96 (4)
C11—C12	1.556 (4)	C28—H28B	1.01 (4)
C11—H11	0.98 (3)	C28—H28C	1.04 (4)
C12—C13	1.524 (4)	O29—H29	0.84 (4)
C12—C19	1.550 (4)	O30—H30	0.84 (4)

C2L—O1L—H1L	108 (3)	C14—C13—H13A	109.8 (17)
O1L—C2L—H2L	109 (2)	C12—C13—H13B	109.1 (18)
O1L—C2L—H3L	112 (2)	C14—C13—H13B	111.1 (18)
H2L—C2L—H3L	111 (3)	H13A—C13—H13B	106 (2)
O1L—C2L—H4L	111 (2)	C13—C14—C6	114.2 (2)
H2L—C2L—H4L	107 (3)	C13—C14—H14A	109 (2)
H3L—C2L—H4L	108 (3)	C6—C14—H14A	109 (2)
H1W—O1W—H2W	108 (4)	C13—C14—H14B	112 (2)
C16—C1—C2	108.0 (3)	C6—C14—H14B	108 (2)
C16—C1—C15	107.3 (3)	H14A—C14—H14B	105 (3)
C2—C1—C15	110.0 (3)	C1—C15—H15A	111 (3)
C16—C1—C6	108.3 (3)	C1—C15—H15B	108 (3)
C2—C1—C6	107.6 (2)	H15A—C15—H15B	105 (4)
C15—C1—C6	115.4 (3)	C1—C15—H15C	109 (3)
O30—C2—C3	111.9 (2)	H15A—C15—H15C	111 (4)
O30—C2—C1	109.6 (2)	H15B—C15—H15C	113 (4)
C3—C2—C1	112.6 (2)	C1—C16—H16A	112 (2)
O30—C2—H2	109.1 (17)	C1—C16—H16B	109 (2)
C3—C2—H2	107.2 (17)	H16A—C16—H16B	108 (3)
C1—C2—H2	106.2 (17)	C1—C16—H16C	107 (2)

O29—C3—C4	110.5 (2)	H16A—C16—H16C	113 (3)
O29—C3—C2	111.6 (2)	H16B—C16—H16C	109 (3)
C4—C3—C2	110.2 (2)	C5—C17—H17A	108 (2)
O29—C3—H3	103.7 (18)	C5—C17—H17B	113 (2)
C4—C3—H3	111.9 (17)	H17A—C17—H17B	104 (3)
C2—C3—H3	108.8 (18)	C5—C17—H17C	111 (2)
C3—C4—C5	114.3 (2)	H17A—C17—H17C	112 (3)
C3—C4—H4A	108.3 (19)	H17B—C17—H17C	109 (3)
C5—C4—H4A	107.3 (19)	C10—C18—H18A	113 (2)
C3—C4—H4B	108.9 (18)	C10—C18—H18B	111 (2)
C5—C4—H4B	111.6 (18)	H18A—C18—H18B	105 (3)
H4A—C4—H4B	106 (3)	C10—C18—H18C	113 (2)
C4—C5—C6	108.2 (2)	H18A—C18—H18C	105 (3)
C4—C5—C17	108.0 (3)	H18B—C18—H18C	109 (3)
C6—C5—C17	113.2 (2)	C12—C19—H19A	109 (2)
C4—C5—C7	111.3 (2)	C12—C19—H19B	114 (2)
C6—C5—C7	109.1 (2)	H19A—C19—H19B	105 (3)
C17—C5—C7	107.0 (2)	C12—C19—H19C	112 (2)
C5—C6—C14	112.9 (2)	H19A—C19—H19C	105 (3)
C5—C6—C1	118.1 (2)	H19B—C19—H19C	110 (3)
C14—C6—C1	112.2 (2)	C21—C20—C11	115.1 (2)
C5—C6—H6	104.9 (16)	C21—C20—H20A	109.4 (17)
C14—C6—H6	105.4 (16)	C11—C20—H20A	109.4 (17)
C1—C6—H6	101.4 (16)	C21—C20—H20B	106.2 (17)
C8—C7—C12	108.6 (2)	C11—C20—H20B	110.8 (17)
C8—C7—C5	116.7 (2)	H20A—C20—H20B	105 (2)
C12—C7—C5	116.6 (2)	O27—C21—C20	108.3 (2)
C8—C7—H7	104.4 (16)	O27—C21—C22	109.8 (2)
C12—C7—H7	104.5 (16)	C20—C21—C22	112.3 (2)
C5—C7—H7	104.3 (16)	O27—C21—H21	110.3 (18)
C9—C8—C7	110.0 (2)	C20—C21—H21	109.2 (18)
C9—C8—H8A	106.7 (19)	C22—C21—H21	106.9 (18)
C7—C8—H8A	111.4 (19)	N26—C22—C23	109.8 (2)
C9—C8—H8B	112.6 (19)	N26—C22—C21	110.3 (2)
C7—C8—H8B	111.8 (19)	C23—C22—C21	111.4 (2)
H8A—C8—H8B	104 (3)	N26—C22—H22	107.5 (18)
C10—C9—C8	124.8 (3)	C23—C22—H22	109.3 (19)
C10—C9—H9	120 (2)	C21—C22—H22	108.5 (19)
C8—C9—H9	115 (2)	O24—C23—O25	126.8 (3)
C9—C10—C18	121.4 (3)	O24—C23—C22	117.5 (3)
C9—C10—C11	122.3 (3)	O25—C23—C22	115.6 (2)
C18—C10—C11	116.4 (3)	C22—N26—H26A	108 (2)
C10—C11—C20	109.9 (2)	C22—N26—H26B	108 (3)
C10—C11—C12	110.8 (2)	H26A—N26—H26B	106 (3)
C20—C11—C12	115.9 (2)	C22—N26—H26C	112 (2)
C10—C11—H11	104.1 (17)	H26A—N26—H26C	113 (3)
C20—C11—H11	105.4 (17)	H26B—N26—H26C	109 (3)
C12—C11—H11	110.0 (17)	C21—O27—C28	113.8 (2)

C13—C12—C19	108.4 (2)	O27—C28—H28A	112 (2)
C13—C12—C11	113.1 (2)	O27—C28—H28B	106 (2)
C19—C12—C11	106.0 (2)	H28A—C28—H28B	112 (3)
C13—C12—C7	108.1 (2)	O27—C28—H28C	106 (2)
C19—C12—C7	114.7 (2)	H28A—C28—H28C	108 (3)
C11—C12—C7	106.6 (2)	H28B—C28—H28C	112 (3)
C12—C13—C14	112.4 (2)	C3—O29—H29	113 (3)
C12—C13—H13A	107.9 (17)	C2—O30—H30	108 (3)

C16—C1—C2—O30	−63.7 (3)	C8—C9—C10—C11	−3.1 (5)
C15—C1—C2—O30	53.2 (3)	C9—C10—C11—C20	113.1 (3)
C6—C1—C2—O30	179.6 (3)	C18—C10—C11—C20	−68.2 (3)
C16—C1—C2—C3	171.1 (3)	C9—C10—C11—C12	−16.2 (4)
C15—C1—C2—C3	−72.1 (3)	C18—C10—C11—C12	162.5 (2)
C6—C1—C2—C3	54.4 (3)	C10—C11—C12—C13	169.4 (2)
O30—C2—C3—O29	53.1 (3)	C20—C11—C12—C13	43.3 (3)
C1—C2—C3—O29	177.1 (2)	C10—C11—C12—C19	−72.0 (3)
O30—C2—C3—C4	176.3 (2)	C20—C11—C12—C19	161.9 (2)
C1—C2—C3—C4	−59.7 (3)	C10—C11—C12—C7	50.6 (3)
O29—C3—C4—C5	−178.3 (2)	C20—C11—C12—C7	−75.5 (3)
C2—C3—C4—C5	57.8 (3)	C8—C7—C12—C13	168.6 (2)
C3—C4—C5—C6	−50.5 (3)	C5—C7—C12—C13	34.1 (3)
C3—C4—C5—C17	72.4 (3)	C8—C7—C12—C19	47.4 (3)
C3—C4—C5—C7	−170.4 (2)	C5—C7—C12—C19	−87.0 (3)
C4—C5—C6—C14	−177.9 (2)	C8—C7—C12—C11	−69.5 (3)
C17—C5—C6—C14	62.4 (3)	C5—C7—C12—C11	156.1 (2)
C7—C5—C6—C14	−56.6 (3)	C19—C12—C13—C14	62.3 (3)
C4—C5—C6—C1	48.4 (3)	C11—C12—C13—C14	179.5 (3)
C17—C5—C6—C1	−71.3 (3)	C7—C12—C13—C14	−62.7 (3)
C7—C5—C6—C1	169.7 (2)	C12—C13—C14—C6	30.8 (4)
C16—C1—C6—C5	−167.2 (3)	C5—C6—C14—C13	30.5 (4)
C2—C1—C6—C5	−50.7 (3)	C1—C6—C14—C13	167.0 (3)
C15—C1—C6—C5	72.5 (4)	C10—C11—C20—C21	143.4 (2)
C16—C1—C6—C14	58.8 (3)	C12—C11—C20—C21	−90.1 (3)
C2—C1—C6—C14	175.3 (3)	C11—C20—C21—O27	−60.9 (3)
C15—C1—C6—C14	−61.5 (4)	C11—C20—C21—C22	177.6 (2)
C4—C5—C7—C8	11.8 (3)	O27—C21—C22—N26	−41.8 (3)
C6—C5—C7—C8	−107.5 (3)	C20—C21—C22—N26	78.8 (3)
C17—C5—C7—C8	129.6 (3)	O27—C21—C22—C23	−164.0 (2)
C4—C5—C7—C12	142.5 (2)	C20—C21—C22—C23	−43.4 (3)
C6—C5—C7—C12	23.2 (3)	N26—C22—C23—O24	−8.9 (3)
C17—C5—C7—C12	−99.6 (3)	C21—C22—C23—O24	113.6 (3)
C12—C7—C8—C9	50.1 (3)	N26—C22—C23—O25	172.5 (2)
C5—C7—C8—C9	−175.5 (2)	C21—C22—C23—O25	−65.0 (3)
C7—C8—C9—C10	−14.5 (4)	C20—C21—O27—C28	154.3 (2)
C8—C9—C10—C18	178.3 (3)	C22—C21—O27—C28	−82.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*L*—H1*L*···O25	0.86 (4)	1.81 (4)	2.662 (3)	171 (4)
O1*W*—H1*W*···O29^{i}	0.87 (4)	1.92 (4)	2.767 (3)	162 (4)
O1*W*—H2*W*···O1*L*^{ii}	0.83 (4)	2.15 (4)	2.948 (3)	162 (4)
C20—H20*B*···O1*W*	0.99 (3)	2.47 (3)	3.423 (3)	162 (2)
C22—H22···O24^{iii}	0.93 (3)	2.54 (3)	3.385 (3)	151 (3)
N26—H26*A*···O30^{iv}	0.92 (4)	2.24 (4)	2.846 (3)	123 (3)
N26—H26*B*···O1*L*^{v}	0.92 (4)	1.95 (4)	2.869 (3)	172 (4)
N26—H26*C*···O1*W*	0.86 (4)	1.95 (4)	2.798 (3)	169 (3)
C28—H28*A*···O30^{iv}	0.96 (4)	2.51 (4)	3.346 (4)	144 (3)
O29—H29···O25^{vi}	0.84 (4)	1.97 (4)	2.769 (3)	157 (4)
O30—H30···O24^{vi}	0.84 (4)	1.85 (4)	2.680 (3)	171 (4)

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