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(1′*S*,2*R*,3*S*,4*S*)-Ethyl 2-hydroxy-4-methyl-3-(1′-phenylethylcarbamoyl)hexanoate

Oleg I. Larionov,[a] Armin de Meijere,[a] Dmitry S. Yufit[b]* and Judith A. K. Howard[b]

[a]Institut für Organische und Biomolekulare Chemie der Georg-August-Universität Göttingen, Tammannstraße 2, D-37077 Göttingen, Germany, and [b]Chemistry Department, University of Durham, South Rd, Durham DH1 3LE, England

Correspondence e-mail: d.s.yufit@durham.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.050
wR factor = 0.126
Data-to-parameter ratio = 11.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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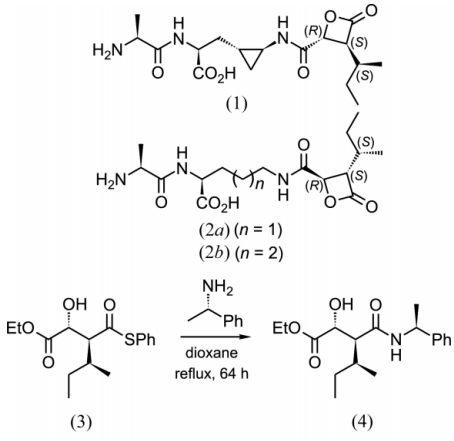
The relative configuration of the title compound, $C_{18}H_{27}NO_4$, was determined as being *R,S,S,S*. There are three crystallographically independent molecules in the asymmetric unit, which show only slight conformational differences. Molecules in the crystal structure are connected by hydrogen bonds in ribbons along the *a* axis.

Comment

Appropriate derivatives of the new natural products belactosins A, (1), C, (2*a*), and its homo-analogue, (2*b*) (see scheme), are highly active proteasome inhibitors (Asai *et al.*, 2000, 2004, Mizukami *et al.*, 1997), which show an impressive potential against some types of cancer and inflammatory diseases (Gillessen *et al.*, 2002; Almond & Cohen, 2002; Elliot *et al.*, 2003). In continuation of our search for synthetic approaches to enantioselective total syntheses of belactosins (Brandl *et al.*, 2000) a precursor of the β-lactone moiety (3) was prepared (Larionov & de Meijere, 2004). The absolute configuration of the β-lactone cycle of the natural products (1)–(3) is (2*R*,3*S*,4*S*), so it was crucial to establish the relative configuration of these centres in (3). Unfortunately, compound (3) is liquid under ambient conditions and a crystalline derivative of (3) had to be prepared. After some experiments, the solid amide (4) was obtained by the reaction of (3) with (*S*)-α-phenylethylamine (see scheme). The X-ray crystal structure of amide (4) is reported in this paper.



There are three independent molecules of (4) in the asymmetric unit (Fig. 1). They all have the same configuration at their chiral centres, but differ by the orientation of the ethyl groups (C11) and phenyl rings (Fig. 2). The absolute configuration of the compound was assigned on the basis of the known *S* configuration of the α-phenylethylamine, used in the

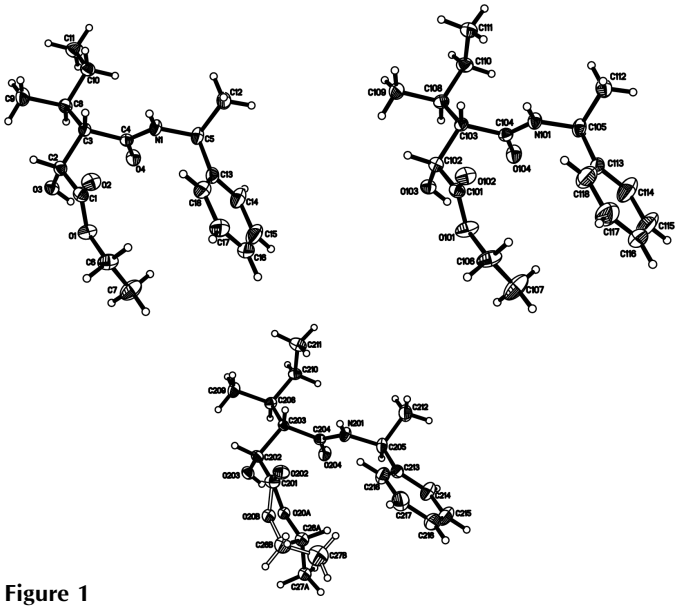


Figure 1
The molecular structure of the three independent molecules of (4) and the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

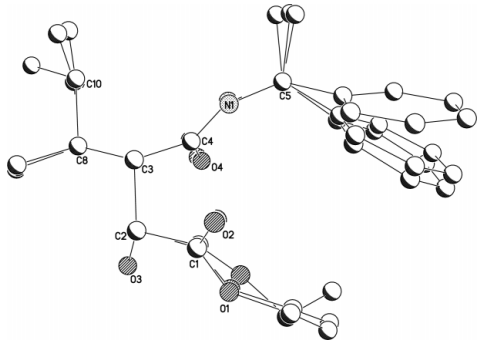


Figure 2
A least-squares superposition of the independent molecules. H atoms and one of the disordered ethoxy groups have been omitted for clarity.

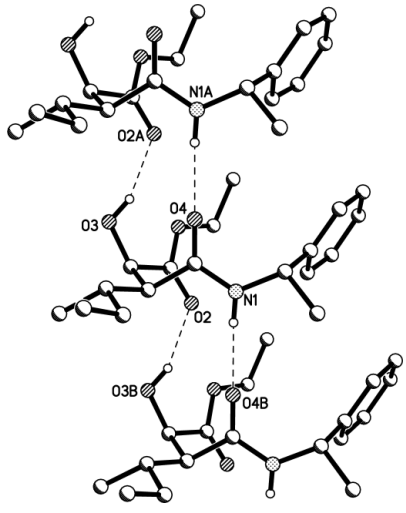


Figure 3
Fragment of the hydrogen-bonded ribbon in the structure of (4). Suffixes *A* and *B* correspond to symmetry codes (ii) and (i), respectively, in Table 1.

synthesis of (4). The terminal ethoxy group of one of the molecules is disordered over two positions; the atoms of the

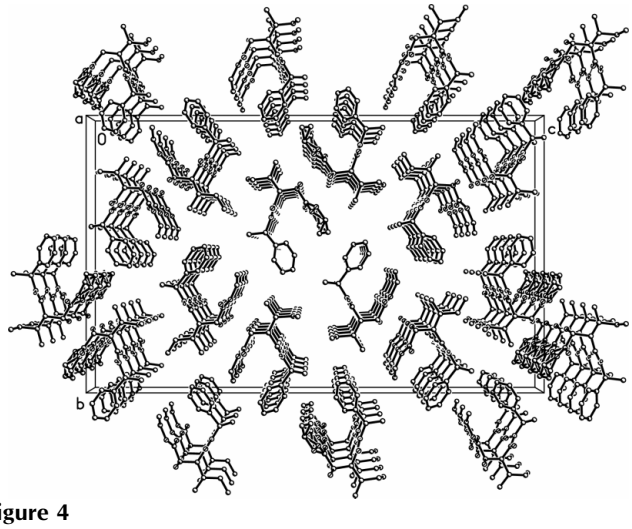


Figure 4
Packing of the molecules (4) in the crystal structure, viewed along the *a* axis, H atoms have been omitted for clarity.

ethoxy groups in the other two molecules also show high anisotropic displacement parameters and are probably also slightly disordered. The molecular geometry of (4) does not reveal any remarkable features. In the crystal structure, the molecules are linked together by pairs of strong O1—H···O2 and N1—H···O4 hydrogen bonds (Fig. 3 and Table 1), forming ribbons which are parallel to the **a** direction (Fig. 4). Each ribbon is composed of one of the crystallographically independent molecules and its symmetry-equivalents.

Experimental

Crystals of (4) suitable for the X-ray experiment were obtained by slow evaporation of a solution in EtOAc–hexane

Crystal data

$C_{18}H_{27}NO_4$
M_r = 321.41
Orthorhombic, $P2_12_12_1$
a = 5.04730 (1) Å
b = 25.1504 (5) Å
c = 41.4912 (9) Å
V = 5266.96 (19) Å^3
Z = 12
D_x = 1.216 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7902 reflections
θ = 2.5–29.1°
μ = 0.09 mm^{-1}
T = 120 (2) K
Prism, colourless
0.46 × 0.16 × 0.14 mm

Data collection

Bruker SMART 6000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.988
44 787 measured reflections
7254 independent reflections
6485 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 28.0°
$h = -6 \rightarrow 6$
$k = -31 \rightarrow 33$
$l = -54 \rightarrow 54$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.126
S = 1.15
7254 reflections
628 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 2.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O4^{i}	0.88	2.10	2.978 (3)	176
O3—H3···O2^{ii}	0.84 (4)	2.02 (4)	2.809 (3)	156 (3)
N101—H10C···O104^{i}	0.88	2.10	2.977 (3)	176
O103—H10D···O102^{ii}	0.80 (4)	2.08 (4)	2.808 (3)	152 (4)
N201—H20A···O204^{ii}	0.88	2.13	3.004 (3)	175
O203—H20B···O202^{i}	0.75 (4)	2.09 (4)	2.795 (3)	158 (4)

Symmetry codes: (i) $1+x, y, z$; (ii) $x-1, y, z$.

All H atoms were located in difference Fourier maps and included in the refinement in the riding mode, with isotropic displacement parameters of 1.5 (H atoms of methyl groups) and 1.2 (all other H atoms) times U_{eq} of the parent atom. H atoms of oxy groups were refined freely with U_{iso} equal $1.5U_{eq}$ of corresponding O atom. In the absence of significant anomalous scattering effects, Friedel pairs have been merged. The absolute configuration can not be determined from the diffraction data, but is known from the synthesis and has been assumed in the refinement.

Data collection: *SMART* (Bruker, 1998–2000); cell refinement: *SAINT* (Bruker, 1998–2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998–2000); software used to prepare material for publication: *SHELXTL*.

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supporting information

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Cell parameters from 7902 reflections
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$\theta_{max} = 28.0°$, $\theta_{min} = 1.7°$
$h = -6 \rightarrow 6$
$k = -31 \rightarrow 33$
$l = -54 \rightarrow 54$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.126$
$S = 1.15$
7254 reflections
628 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 2.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1	0.3822 (5)	0.33693 (8)	0.27539 (5)	0.0225 (5)	
H1A	0.5498	0.3285	0.2725	0.027*	
O1	0.1320 (4)	0.34073 (7)	0.18010 (5)	0.0275 (4)	
O2	0.5491 (4)	0.32734 (8)	0.19695 (5)	0.0298 (4)	
O3	−0.0491 (4)	0.25070 (7)	0.20291 (4)	0.0235 (4)	
H3	−0.148 (8)	0.2771 (13)	0.2062 (8)	0.035*	
O4	−0.0439 (4)	0.31388 (8)	0.26634 (5)	0.0280 (4)	
C1	0.3222 (6)	0.31303 (10)	0.19452 (6)	0.0228 (5)	
C2	0.2197 (5)	0.26081 (10)	0.20859 (6)	0.0212 (5)	
H2A	0.3194	0.2319	0.1973	0.025*	
C3	0.2978 (5)	0.25684 (9)	0.24486 (5)	0.0188 (5)	
H3B	0.4955	0.2566	0.2464	0.023*	
C4	0.1946 (6)	0.30488 (9)	0.26314 (6)	0.0194 (5)	
C5	0.3172 (6)	0.38537 (9)	0.29330 (7)	0.0250 (6)	
H5A	0.1417	0.3800	0.3040	0.030*	
C6	0.2094 (7)	0.39134 (11)	0.16579 (7)	0.0308 (6)	
H6A	0.2672	0.3860	0.1432	0.037*	
H6B	0.3577	0.4073	0.1781	0.037*	
C7	−0.0274 (7)	0.42687 (12)	0.16693 (9)	0.0432 (8)	
H7A	0.0172	0.4614	0.1574	0.065*	
H7B	−0.0821	0.4319	0.1894	0.065*	
H7C	−0.1728	0.4106	0.1548	0.065*	
C8	0.1925 (6)	0.20473 (9)	0.25960 (6)	0.0235 (5)	
H8A	−0.0055	0.2053	0.2588	0.028*	
C9	0.2909 (9)	0.15699 (11)	0.24007 (7)	0.0416 (8)	
H9A	0.2200	0.1241	0.2494	0.062*	
H9B	0.4850	0.1559	0.2406	0.062*	
H9C	0.2309	0.1603	0.2177	0.062*	
C10	0.2785 (6)	0.20000 (10)	0.29489 (6)	0.0258 (6)	
H10A	0.4731	0.1953	0.2957	0.031*	
H10B	0.2354	0.2336	0.3062	0.031*	
C11	0.1469 (7)	0.15378 (11)	0.31277 (7)	0.0365 (7)	
H11A	0.2112	0.1527	0.3350	0.055*	
H11B	0.1908	0.1203	0.3020	0.055*	
H11C	−0.0457	0.1587	0.3127	0.055*	
C12	0.5248 (7)	0.39418 (10)	0.31949 (6)	0.0300 (6)	
H12A	0.5337	0.3627	0.3334	0.045*	
H12B	0.4760	0.4253	0.3324	0.045*	
H12C	0.6981	0.4002	0.3095	0.045*	
C13	0.2959 (6)	0.43376 (10)	0.27136 (7)	0.0275 (6)	

C14	0.1061 (7)	0.47243 (11)	0.27796 (8)	0.0380 (7)
H14A	−0.0128	0.4676	0.2955	0.046*
C15	0.0893 (8)	0.51818 (12)	0.25909 (9)	0.0445 (9)
H15A	−0.0429	0.5440	0.2636	0.053*
C16	0.2618 (8)	0.52608 (12)	0.23413 (8)	0.0427 (9)
H16A	0.2501	0.5574	0.2214	0.051*
C17	0.4528 (9)	0.48842 (12)	0.22753 (7)	0.0430 (8)
H17A	0.5744	0.4940	0.2104	0.052*
C18	0.4679 (7)	0.44212 (11)	0.24595 (7)	0.0356 (7)
H18A	0.5978	0.4161	0.2410	0.043*
N101	0.8835 (5)	0.15101 (8)	0.06687 (5)	0.0236 (5)
H10C	1.0509	0.1590	0.0703	0.028*
O101	0.6361 (4)	0.14903 (8)	0.16018 (5)	0.0326 (5)
O102	1.0569 (4)	0.16332 (8)	0.14527 (5)	0.0290 (4)
O103	0.4582 (4)	0.23984 (8)	0.13859 (4)	0.0235 (4)
H10D	0.384 (8)	0.2117 (14)	0.1376 (8)	0.035*
O104	0.4568 (4)	0.17515 (8)	0.07524 (5)	0.0309 (5)
C101	0.8274 (6)	0.17727 (10)	0.14689 (6)	0.0224 (5)
C102	0.7274 (5)	0.22945 (10)	0.13252 (6)	0.0203 (5)
H10E	0.8294	0.2585	0.1434	0.024*
C103	0.8012 (5)	0.23210 (9)	0.09624 (5)	0.0186 (5)
H10F	0.9988	0.2322	0.0945	0.022*
C104	0.6976 (6)	0.18379 (10)	0.07836 (6)	0.0209 (5)
C105	0.8221 (6)	0.10266 (10)	0.04891 (7)	0.0268 (6)
H10G	0.6402	0.1066	0.0397	0.032*
C106	0.7105 (7)	0.09815 (12)	0.17419 (8)	0.0367 (7)
H10H	0.7613	0.1028	0.1971	0.044*
H10I	0.8629	0.0828	0.1624	0.044*
C107	0.4764 (8)	0.06255 (13)	0.17159 (11)	0.0525 (10)
H10J	0.5195	0.0277	0.1808	0.079*
H10K	0.4281	0.0583	0.1489	0.079*
H10L	0.3272	0.0781	0.1834	0.079*
C108	0.6967 (6)	0.28418 (9)	0.08161 (6)	0.0231 (5)
H10M	0.5001	0.2845	0.0846	0.028*
C109	0.8085 (7)	0.33209 (10)	0.10007 (7)	0.0320 (7)
H10N	0.7711	0.3280	0.1231	0.048*
H10O	0.7253	0.3648	0.0921	0.048*
H10P	1.0005	0.3341	0.0967	0.048*
C110	0.7507 (7)	0.28835 (11)	0.04522 (6)	0.0295 (6)
H11D	0.6654	0.2577	0.0344	0.035*
H11E	0.6647	0.3211	0.0370	0.035*
C111	1.0408 (7)	0.28958 (12)	0.03554 (7)	0.0321 (7)
H11F	1.0546	0.2921	0.0120	0.048*
H11G	1.1279	0.2569	0.0429	0.048*
H11H	1.1270	0.3204	0.0454	0.048*
C112	1.0146 (7)	0.09718 (11)	0.02112 (7)	0.0337 (7)
H11I	1.0091	0.1294	0.0079	0.051*
H11J	0.9650	0.0664	0.0079	0.051*

H11K	1.1942	0.0921	0.0295	0.051*
C113	0.8232 (7)	0.05328 (10)	0.07026 (7)	0.0317 (7)
C114	0.6435 (9)	0.01290 (13)	0.06376 (11)	0.0567 (11)
H11L	0.5151	0.0173	0.0472	0.068*
C115	0.6519 (11)	−0.03393 (14)	0.08150 (13)	0.0696 (14)
H11M	0.5293	−0.0615	0.0769	0.084*
C116	0.8344 (11)	−0.04088 (13)	0.10558 (10)	0.0596 (13)
H11N	0.8375	−0.0729	0.1177	0.071*
C117	1.0115 (12)	−0.00129 (14)	0.11188 (9)	0.0647 (14)
H11O	1.1396	−0.0058	0.1284	0.078*
C118	1.0057 (10)	0.04605 (13)	0.09412 (8)	0.0518 (10)
H11P	1.1300	0.0734	0.0987	0.062*
N201	0.3250 (5)	0.62781 (8)	0.09267 (5)	0.0228 (5)
H20A	0.1569	0.6359	0.0899	0.027*
O202	0.1182 (4)	0.66401 (8)	0.02094 (5)	0.0276 (4)
O203	0.7172 (4)	0.73888 (8)	0.03092 (4)	0.0254 (4)
H20B	0.799 (8)	0.7141 (14)	0.0312 (9)	0.038*
O204	0.7489 (4)	0.65686 (7)	0.08817 (5)	0.0261 (4)
C201	0.3437 (6)	0.67877 (11)	0.01936 (6)	0.0262 (6)
C202	0.4524 (6)	0.72628 (10)	0.03793 (6)	0.0215 (5)
H20C	0.3445	0.7577	0.0312	0.026*
C203	0.3988 (5)	0.71817 (9)	0.07456 (5)	0.0170 (5)
H20D	0.2029	0.7184	0.0781	0.020*
C204	0.5082 (5)	0.66473 (9)	0.08594 (6)	0.0186 (5)
C205	0.3926 (6)	0.57459 (9)	0.10438 (6)	0.0250 (5)
H20E	0.5900	0.5712	0.1041	0.030*
C208	0.5218 (6)	0.76359 (9)	0.09442 (6)	0.0205 (5)
H20J	0.7176	0.7623	0.0909	0.025*
C209	0.4250 (8)	0.81775 (10)	0.08256 (7)	0.0340 (7)
H20K	0.5056	0.8459	0.0956	0.051*
H20L	0.2317	0.8196	0.0845	0.051*
H20M	0.4756	0.8225	0.0599	0.051*
C210	0.4737 (6)	0.75677 (10)	0.13086 (6)	0.0234 (5)
H21A	0.5375	0.7211	0.1373	0.028*
H21B	0.5823	0.7834	0.1425	0.028*
C211	0.1889 (6)	0.76257 (13)	0.14173 (7)	0.0331 (6)
H21C	0.1785	0.7574	0.1651	0.050*
H21D	0.0793	0.7359	0.1309	0.050*
H21E	0.1246	0.7982	0.1362	0.050*
C212	0.3004 (8)	0.56869 (11)	0.13934 (7)	0.0381 (8)
H21F	0.3779	0.5971	0.1524	0.057*
H21G	0.3576	0.5341	0.1477	0.057*
H21H	0.1067	0.5710	0.1402	0.057*
C213	0.2796 (6)	0.53063 (10)	0.08326 (6)	0.0254 (6)
C214	0.3824 (7)	0.47954 (11)	0.08656 (8)	0.0364 (7)
H21I	0.5238	0.4733	0.1012	0.044*
C215	0.2795 (8)	0.43737 (12)	0.06853 (9)	0.0442 (8)
H21J	0.3529	0.4028	0.0707	0.053*

C216	0.0729 (8)	0.44575 (12)	0.04767 (8)	0.0410 (8)	
H21K	0.0024	0.4170	0.0356	0.049*	
C217	−0.0312 (8)	0.49571 (12)	0.04436 (8)	0.0406 (8)	
H21L	−0.1750	0.5014	0.0300	0.049*	
C218	0.0715 (7)	0.53857 (11)	0.06186 (7)	0.0326 (7)	
H21M	−0.0010	0.5731	0.0591	0.039*	
O20A	0.5241 (8)	0.64633 (15)	0.00678 (9)	0.0199 (8)*	0.50
C26A	0.4361 (12)	0.5982 (2)	−0.00926 (13)	0.0252 (11)*	0.50
H26A	0.2928	0.6065	−0.0248	0.030*	0.50
H26B	0.3676	0.5724	0.0067	0.030*	0.50
C27A	0.6712 (11)	0.57546 (19)	−0.02661 (12)	0.0225 (10)*	0.50
H27A	0.6275	0.5399	−0.0346	0.034*	0.50
H27B	0.8216	0.5731	−0.0117	0.034*	0.50
H27C	0.7181	0.5985	−0.0448	0.034*	0.50
O20B	0.5304 (9)	0.66318 (16)	−0.00234 (9)	0.0249 (8)*	0.50
C26B	0.4535 (15)	0.6177 (2)	−0.02181 (15)	0.0358 (13)*	0.50
H26C	0.5068	0.6233	−0.0445	0.043*	0.50
H26D	0.2589	0.6129	−0.0211	0.043*	0.50
C27B	0.585 (2)	0.5708 (3)	−0.0089 (2)	0.0565 (19)*	0.50
H27D	0.5512	0.5403	−0.0231	0.085*	0.50
H27E	0.5156	0.5631	0.0127	0.085*	0.50
H27F	0.7759	0.5772	−0.0076	0.085*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0176 (12)	0.0185 (9)	0.0314 (11)	0.0008 (9)	0.0011 (9)	−0.0070 (8)
O1	0.0193 (10)	0.0277 (9)	0.0355 (10)	−0.0031 (8)	−0.0016 (9)	0.0093 (8)
O2	0.0192 (11)	0.0322 (10)	0.0379 (10)	−0.0036 (9)	−0.0022 (9)	0.0035 (8)
O3	0.0210 (10)	0.0249 (9)	0.0247 (8)	−0.0042 (8)	−0.0026 (8)	−0.0001 (7)
O4	0.0158 (10)	0.0326 (10)	0.0356 (10)	0.0021 (8)	−0.0012 (8)	−0.0081 (8)
C1	0.0221 (14)	0.0279 (12)	0.0183 (10)	−0.0004 (11)	0.0027 (10)	−0.0001 (9)
C2	0.0189 (13)	0.0225 (11)	0.0222 (11)	0.0002 (10)	−0.0004 (10)	−0.0031 (9)
C3	0.0159 (12)	0.0183 (10)	0.0223 (11)	−0.0006 (9)	−0.0011 (10)	−0.0023 (8)
C4	0.0195 (13)	0.0199 (11)	0.0187 (10)	0.0000 (10)	0.0002 (10)	0.0011 (8)
C5	0.0217 (14)	0.0201 (11)	0.0331 (13)	−0.0004 (11)	0.0031 (12)	−0.0073 (10)
C6	0.0252 (16)	0.0317 (13)	0.0354 (14)	−0.0059 (12)	−0.0001 (13)	0.0123 (11)
C7	0.0345 (19)	0.0294 (15)	0.066 (2)	−0.0027 (14)	0.0018 (17)	0.0091 (14)
C8	0.0260 (14)	0.0196 (11)	0.0249 (11)	−0.0055 (11)	−0.0033 (11)	0.0008 (9)
C9	0.068 (3)	0.0223 (12)	0.0345 (14)	0.0003 (16)	−0.0063 (17)	−0.0054 (11)
C10	0.0262 (15)	0.0253 (12)	0.0259 (12)	−0.0022 (11)	−0.0052 (12)	0.0018 (10)
C11	0.042 (2)	0.0320 (14)	0.0352 (14)	−0.0062 (14)	−0.0057 (14)	0.0097 (12)
C12	0.0390 (18)	0.0240 (12)	0.0271 (12)	−0.0015 (13)	−0.0015 (13)	−0.0037 (10)
C13	0.0263 (15)	0.0218 (11)	0.0344 (13)	0.0006 (11)	−0.0088 (12)	−0.0071 (10)
C14	0.0346 (18)	0.0251 (13)	0.0542 (18)	0.0029 (13)	−0.0001 (16)	−0.0072 (12)
C15	0.040 (2)	0.0247 (13)	0.068 (2)	0.0095 (14)	−0.0108 (19)	−0.0073 (14)
C16	0.057 (2)	0.0266 (14)	0.0445 (17)	0.0042 (15)	−0.0259 (18)	−0.0013 (12)
C17	0.061 (2)	0.0355 (15)	0.0323 (14)	0.0030 (17)	−0.0034 (17)	0.0047 (12)

C18	0.0433 (19)	0.0287 (13)	0.0347 (14)	0.0090 (14)	−0.0020 (14)	−0.0016 (11)
N101	0.0178 (12)	0.0226 (10)	0.0304 (11)	−0.0016 (9)	−0.0009 (10)	−0.0061 (8)
O101	0.0196 (11)	0.0316 (10)	0.0464 (11)	0.0040 (9)	−0.0005 (9)	0.0190 (9)
O102	0.0188 (10)	0.0318 (10)	0.0362 (10)	0.0043 (8)	0.0006 (9)	0.0066 (8)
O103	0.0209 (10)	0.0249 (9)	0.0249 (9)	0.0029 (8)	0.0024 (8)	0.0016 (7)
O104	0.0179 (10)	0.0344 (10)	0.0404 (11)	−0.0030 (9)	−0.0017 (9)	−0.0106 (9)
C101	0.0224 (14)	0.0265 (12)	0.0184 (10)	0.0005 (11)	−0.0010 (10)	0.0016 (9)
C102	0.0168 (13)	0.0226 (11)	0.0214 (11)	0.0013 (10)	−0.0019 (10)	0.0007 (9)
C103	0.0167 (12)	0.0192 (10)	0.0199 (10)	−0.0020 (10)	−0.0007 (10)	0.0006 (8)
C104	0.0203 (14)	0.0219 (11)	0.0206 (11)	−0.0024 (10)	0.0006 (10)	0.0013 (9)
C105	0.0206 (14)	0.0239 (12)	0.0360 (14)	−0.0036 (11)	−0.0030 (12)	−0.0087 (10)
C106	0.0253 (16)	0.0336 (14)	0.0511 (17)	0.0049 (13)	0.0017 (15)	0.0220 (13)
C107	0.036 (2)	0.0268 (15)	0.095 (3)	0.0001 (15)	−0.013 (2)	0.0127 (16)
C108	0.0233 (14)	0.0229 (11)	0.0232 (11)	−0.0001 (11)	−0.0011 (11)	0.0038 (9)
C109	0.0438 (19)	0.0210 (12)	0.0312 (13)	0.0001 (13)	0.0029 (14)	0.0000 (10)
C110	0.0337 (17)	0.0328 (13)	0.0220 (12)	−0.0038 (13)	−0.0013 (12)	0.0049 (10)
C111	0.0386 (18)	0.0318 (14)	0.0260 (13)	−0.0027 (13)	0.0057 (13)	0.0027 (11)
C112	0.0405 (19)	0.0306 (13)	0.0299 (13)	−0.0016 (14)	0.0002 (14)	−0.0052 (11)
C113	0.0313 (17)	0.0220 (12)	0.0417 (15)	−0.0043 (12)	0.0135 (14)	−0.0088 (11)
C114	0.047 (2)	0.0314 (16)	0.091 (3)	−0.0123 (17)	0.002 (2)	−0.0050 (17)
C115	0.067 (3)	0.0274 (16)	0.114 (4)	−0.0155 (19)	0.025 (3)	−0.001 (2)
C116	0.095 (4)	0.0261 (15)	0.058 (2)	−0.004 (2)	0.033 (3)	0.0026 (14)
C117	0.109 (4)	0.0406 (18)	0.0444 (19)	−0.009 (2)	−0.003 (3)	0.0078 (15)
C118	0.079 (3)	0.0319 (15)	0.0443 (18)	−0.0142 (19)	−0.007 (2)	0.0035 (13)
N201	0.0170 (11)	0.0173 (9)	0.0343 (11)	0.0011 (9)	−0.0011 (10)	0.0044 (8)
O202	0.0228 (11)	0.0324 (10)	0.0276 (9)	−0.0014 (8)	0.0029 (8)	−0.0033 (8)
O203	0.0238 (11)	0.0287 (9)	0.0237 (8)	0.0021 (8)	0.0041 (8)	0.0045 (7)
O204	0.0162 (10)	0.0251 (9)	0.0370 (10)	0.0016 (8)	−0.0007 (8)	0.0051 (8)
C201	0.0232 (15)	0.0356 (14)	0.0197 (11)	0.0076 (12)	−0.0048 (11)	−0.0017 (10)
C202	0.0211 (14)	0.0262 (12)	0.0172 (10)	0.0025 (11)	0.0006 (10)	0.0019 (9)
C203	0.0153 (12)	0.0188 (10)	0.0168 (10)	−0.0011 (9)	0.0024 (9)	0.0013 (8)
C204	0.0168 (13)	0.0197 (11)	0.0194 (10)	0.0000 (10)	0.0008 (10)	−0.0011 (9)
C205	0.0226 (14)	0.0196 (11)	0.0329 (13)	−0.0015 (11)	−0.0004 (12)	0.0078 (10)
C208	0.0197 (13)	0.0187 (10)	0.0232 (11)	−0.0028 (10)	0.0009 (10)	−0.0018 (9)
C209	0.049 (2)	0.0173 (11)	0.0358 (14)	−0.0006 (13)	0.0020 (15)	0.0019 (10)
C210	0.0241 (14)	0.0258 (12)	0.0202 (11)	0.0006 (11)	−0.0006 (11)	−0.0043 (9)
C211	0.0262 (16)	0.0465 (16)	0.0265 (13)	−0.0020 (14)	0.0034 (12)	−0.0029 (12)
C212	0.054 (2)	0.0274 (13)	0.0323 (14)	−0.0059 (15)	−0.0005 (16)	0.0041 (11)
C213	0.0255 (15)	0.0219 (11)	0.0289 (12)	−0.0002 (11)	0.0084 (12)	0.0021 (9)
C214	0.0327 (18)	0.0236 (12)	0.0530 (18)	0.0032 (13)	−0.0034 (15)	0.0010 (12)
C215	0.045 (2)	0.0221 (13)	0.065 (2)	0.0009 (14)	0.0065 (19)	−0.0050 (13)
C216	0.055 (2)	0.0278 (14)	0.0403 (16)	−0.0108 (16)	0.0065 (17)	−0.0069 (12)
C217	0.050 (2)	0.0364 (15)	0.0354 (15)	−0.0089 (16)	−0.0075 (16)	0.0004 (12)
C218	0.0380 (18)	0.0213 (12)	0.0385 (15)	−0.0022 (13)	0.0013 (14)	0.0008 (11)

Geometric parameters (Å, º)

N1—C4	1.343 (3)	C109—H10P	0.9800
N1—C5	1.464 (3)	C110—C111	1.519 (5)
N1—H1A	0.8800	C110—H11D	0.9900
O1—C1	1.329 (3)	C110—H11E	0.9900
O1—C6	1.458 (3)	C111—H11F	0.9800
O2—C1	1.205 (4)	C111—H11G	0.9800
O3—C2	1.400 (3)	C111—H11H	0.9800
O3—H3	0.84 (4)	C112—H11I	0.9800
O4—C4	1.232 (3)	C112—H11J	0.9800
C1—C2	1.528 (4)	C112—H11K	0.9800
C2—C3	1.559 (3)	C113—C118	1.365 (5)
C2—H2A	1.0000	C113—C114	1.388 (5)
C3—C4	1.519 (3)	C114—C115	1.389 (6)
C3—C8	1.541 (3)	C114—H11L	0.9500
C3—H3B	1.0000	C115—C116	1.370 (7)
C5—C13	1.524 (4)	C115—H11M	0.9500
C5—C12	1.526 (4)	C116—C117	1.363 (6)
C5—H5A	1.0000	C116—H11N	0.9500
C6—C7	1.493 (5)	C117—C118	1.400 (5)
C6—H6A	0.9900	C117—H11O	0.9500
C6—H6B	0.9900	C118—H11P	0.9500
C7—H7A	0.9800	N201—C204	1.340 (3)
C7—H7B	0.9800	N201—C205	1.465 (3)
C7—H7C	0.9800	N201—H20A	0.8800
C8—C9	1.531 (4)	O202—C201	1.199 (4)
C8—C10	1.532 (3)	O203—C202	1.404 (3)
C8—H8A	1.0000	O203—H20B	0.75 (4)
C9—H9A	0.9800	O204—C204	1.234 (3)
C9—H9B	0.9800	C201—O20A	1.330 (5)
C9—H9C	0.9800	C201—O20B	1.361 (5)
C10—C11	1.531 (4)	C201—C202	1.524 (4)
C10—H10A	0.9900	C202—C203	1.557 (3)
C10—H10B	0.9900	C202—H20C	1.0000
C11—H11A	0.9800	C203—C204	1.528 (3)
C11—H11B	0.9800	C203—C208	1.539 (3)
C11—H11C	0.9800	C203—H20D	1.0000
C12—H12A	0.9800	C205—C213	1.522 (4)
C12—H12B	0.9800	C205—C212	1.531 (4)
C12—H12C	0.9800	C205—H20E	1.0000
C13—C18	1.382 (4)	C208—C209	1.528 (3)
C13—C14	1.392 (4)	C208—C210	1.541 (3)
C14—C15	1.394 (5)	C208—H20J	1.0000
C14—H14A	0.9500	C209—H20K	0.9800
C15—C16	1.368 (5)	C209—H20L	0.9800
C15—H15A	0.9500	C209—H20M	0.9800
C16—C17	1.379 (5)	C210—C211	1.513 (4)

C16—H16A	0.9500	C210—H21A	0.9900
C17—C18	1.395 (4)	C210—H21B	0.9900
C17—H17A	0.9500	C211—H21C	0.9800
C18—H18A	0.9500	C211—H21D	0.9800
N101—C104	1.336 (3)	C211—H21E	0.9800
N101—C105	1.459 (3)	C212—H21F	0.9800
N101—H10C	0.8800	C212—H21G	0.9800
O101—C101	1.320 (3)	C212—H21H	0.9800
O101—C106	1.455 (3)	C213—C218	1.390 (4)
O102—C101	1.212 (4)	C213—C214	1.393 (4)
O103—C102	1.406 (3)	C214—C215	1.398 (4)
O103—H10D	0.80 (4)	C214—H21I	0.9500
O104—C104	1.241 (4)	C215—C216	1.371 (5)
C101—C102	1.527 (3)	C215—H21J	0.9500
C102—C103	1.552 (3)	C216—C217	1.369 (5)
C102—H10E	1.0000	C216—H21K	0.9500
C103—C104	1.517 (3)	C217—C218	1.399 (4)
C103—C108	1.537 (3)	C217—H21L	0.9500
C103—H10F	1.0000	C218—H21M	0.9500
C105—C112	1.514 (4)	O20A—C26A	1.450 (6)
C105—C113	1.525 (4)	C26A—C27A	1.502 (8)
C105—H10G	1.0000	C26A—H26A	0.9900
C106—C107	1.486 (5)	C26A—H26B	0.9900
C106—H10H	0.9900	C27A—H27A	0.9800
C106—H10I	0.9900	C27A—H27B	0.9800
C107—H10J	0.9800	C27A—H27C	0.9800
C107—H10K	0.9800	O20B—C26B	1.453 (7)
C107—H10L	0.9800	C26B—C27B	1.455 (10)
C108—C110	1.538 (3)	C26B—H26C	0.9900
C108—C109	1.535 (4)	C26B—H26D	0.9900
C108—H10M	1.0000	C27B—H27D	0.9800
C109—H10N	0.9800	C27B—H27E	0.9800
C109—H10O	0.9800	C27B—H27F	0.9800

C4—N1—C5	122.2 (2)	C111—C110—C108	115.6 (2)
C4—N1—H1A	118.9	C111—C110—H11D	108.4
C5—N1—H1A	118.9	C108—C110—H11D	108.4
C1—O1—C6	116.6 (2)	C111—C110—H11E	108.4
C2—O3—H3	114 (3)	C108—C110—H11E	108.4
O2—C1—O1	124.6 (2)	H11D—C110—H11E	107.4
O2—C1—C2	123.2 (3)	C110—C111—H11F	109.5
O1—C1—C2	112.2 (2)	C110—C111—H11G	109.5
O3—C2—C1	114.8 (2)	H11F—C111—H11G	109.5
O3—C2—C3	113.3 (2)	C110—C111—H11H	109.5
C1—C2—C3	109.8 (2)	H11F—C111—H11H	109.5
O3—C2—H2A	106.1	H11G—C111—H11H	109.5
C1—C2—H2A	106.1	C105—C112—H11I	109.5
C3—C2—H2A	106.1	C105—C112—H11J	109.5

C4—C3—C8	111.1 (2)	H11I—C112—H11J	109.5
C4—C3—C2	110.14 (19)	C105—C112—H11K	109.5
C8—C3—C2	110.51 (19)	H11I—C112—H11K	109.5
C4—C3—H3B	108.3	H11J—C112—H11K	109.5
C8—C3—H3B	108.3	C118—C113—C114	119.0 (3)
C2—C3—H3B	108.3	C118—C113—C105	122.1 (3)
O4—C4—N1	122.5 (2)	C114—C113—C105	118.7 (3)
O4—C4—C3	122.4 (2)	C115—C114—C113	119.8 (4)
N1—C4—C3	115.1 (2)	C115—C114—H11L	120.1
N1—C5—C13	112.2 (2)	C113—C114—H11L	120.1
N1—C5—C12	109.2 (2)	C116—C115—C114	121.0 (4)
C13—C5—C12	111.0 (2)	C116—C115—H11M	119.5
N1—C5—H5A	108.1	C114—C115—H11M	119.5
C13—C5—H5A	108.1	C117—C116—C115	119.2 (3)
C12—C5—H5A	108.1	C117—C116—H11N	120.4
O1—C6—C7	107.2 (2)	C115—C116—H11N	120.4
O1—C6—H6A	110.3	C116—C117—C118	120.4 (4)
C7—C6—H6A	110.3	C116—C117—H11O	119.8
O1—C6—H6B	110.3	C118—C117—H11O	119.8
C7—C6—H6B	110.3	C113—C118—C117	120.6 (4)
H6A—C6—H6B	108.5	C113—C118—H11P	119.7
C6—C7—H7A	109.5	C117—C118—H11P	119.7
C6—C7—H7B	109.5	C204—N201—C205	122.8 (2)
H7A—C7—H7B	109.5	C204—N201—H20A	118.6
C6—C7—H7C	109.5	C205—N201—H20A	118.6
H7A—C7—H7C	109.5	C202—O203—H20B	110 (3)
H7B—C7—H7C	109.5	O202—C201—O20A	118.8 (3)
C9—C8—C10	110.7 (2)	O202—C201—O20B	127.2 (3)
C9—C8—C3	110.2 (2)	O20A—C201—O20B	24.38 (19)
C10—C8—C3	110.3 (2)	O202—C201—C202	123.8 (3)
C9—C8—H8A	108.5	O20A—C201—C202	115.7 (3)
C10—C8—H8A	108.5	O20B—C201—C202	108.1 (3)
C3—C8—H8A	108.5	O203—C202—C201	114.5 (2)
C8—C9—H9A	109.5	O203—C202—C203	113.4 (2)
C8—C9—H9B	109.5	C201—C202—C203	109.2 (2)
H9A—C9—H9B	109.5	O203—C202—H20C	106.4
C8—C9—H9C	109.5	C201—C202—H20C	106.4
H9A—C9—H9C	109.5	C203—C202—H20C	106.4
H9B—C9—H9C	109.5	C204—C203—C208	110.0 (2)
C11—C10—C8	113.5 (2)	C204—C203—C202	110.72 (19)
C11—C10—H10A	108.9	C208—C203—C202	110.81 (19)
C8—C10—H10A	108.9	C204—C203—H20D	108.4
C11—C10—H10B	108.9	C208—C203—H20D	108.4
C8—C10—H10B	108.9	C202—C203—H20D	108.4
H10A—C10—H10B	107.7	O204—C204—N201	123.5 (2)
C10—C11—H11A	109.5	O204—C204—C203	121.3 (2)
C10—C11—H11B	109.5	N201—C204—C203	115.1 (2)
H11A—C11—H11B	109.5	N201—C205—C213	112.7 (2)

C10—C11—H11C	109.5	N201—C205—C212	109.4 (2)
H11A—C11—H11C	109.5	C213—C205—C212	111.2 (2)
H11B—C11—H11C	109.5	N201—C205—H20E	107.8
C5—C12—H12A	109.5	C213—C205—H20E	107.8
C5—C12—H12B	109.5	C212—C205—H20E	107.8
H12A—C12—H12B	109.5	C209—C208—C203	111.1 (2)
C5—C12—H12C	109.5	C209—C208—C210	111.4 (2)
H12A—C12—H12C	109.5	C203—C208—C210	112.3 (2)
H12B—C12—H12C	109.5	C209—C208—H20J	107.3
C18—C13—C14	118.4 (3)	C203—C208—H20J	107.3
C18—C13—C5	122.2 (3)	C210—C208—H20J	107.3
C14—C13—C5	119.3 (3)	C208—C209—H20K	109.5
C15—C14—C13	120.5 (3)	C208—C209—H20L	109.5
C15—C14—H14A	119.7	H20K—C209—H20L	109.5
C13—C14—H14A	119.7	C208—C209—H20M	109.5
C16—C15—C14	120.4 (3)	H20K—C209—H20M	109.5
C16—C15—H15A	119.8	H20L—C209—H20M	109.5
C14—C15—H15A	119.8	C211—C210—C208	115.6 (2)
C15—C16—C17	119.7 (3)	C211—C210—H21A	108.4
C15—C16—H16A	120.1	C208—C210—H21A	108.4
C17—C16—H16A	120.1	C211—C210—H21B	108.4
C16—C17—C18	120.2 (3)	C208—C210—H21B	108.4
C16—C17—H17A	119.9	H21A—C210—H21B	107.5
C18—C17—H17A	119.9	C210—C211—H21C	109.5
C13—C18—C17	120.7 (3)	C210—C211—H21D	109.5
C13—C18—H18A	119.6	H21C—C211—H21D	109.5
C17—C18—H18A	119.6	C210—C211—H21E	109.5
C104—N101—C105	123.2 (2)	H21C—C211—H21E	109.5
C104—N101—H10C	118.4	H21D—C211—H21E	109.5
C105—N101—H10C	118.4	C205—C212—H21F	109.5
C101—O101—C106	116.8 (2)	C205—C212—H21G	109.5
C102—O103—H10D	106 (3)	H21F—C212—H21G	109.5
O102—C101—O101	124.5 (2)	C205—C212—H21H	109.5
O102—C101—C102	122.9 (2)	H21F—C212—H21H	109.5
O101—C101—C102	112.6 (2)	H21G—C212—H21H	109.5
O103—C102—C101	114.2 (2)	C218—C213—C214	118.5 (3)
O103—C102—C103	113.4 (2)	C218—C213—C205	123.2 (2)
C101—C102—C103	109.6 (2)	C214—C213—C205	118.3 (3)
O103—C102—H10E	106.3	C213—C214—C215	120.6 (3)
C101—C102—H10E	106.3	C213—C214—H21I	119.7
C103—C102—H10E	106.3	C215—C214—H21I	119.7
C104—C103—C108	111.8 (2)	C216—C215—C214	120.2 (3)
C104—C103—C102	110.9 (2)	C216—C215—H21J	119.9
C108—C103—C102	109.7 (2)	C214—C215—H21J	119.9
C104—C103—H10F	108.1	C217—C216—C215	119.8 (3)
C108—C103—H10F	108.1	C217—C216—H21K	120.1
C102—C103—H10F	108.1	C215—C216—H21K	120.1
O104—C104—N101	122.8 (2)	C216—C217—C218	120.9 (3)

O104—C104—C103	121.9 (2)	C216—C217—H21L	119.6
N101—C104—C103	115.2 (2)	C218—C217—H21L	119.6
N101—C105—C112	109.2 (2)	C213—C218—C217	120.1 (3)
N101—C105—C113	112.4 (2)	C213—C218—H21M	120.0
C112—C105—C113	111.5 (2)	C217—C218—H21M	120.0
N101—C105—H10G	107.9	C201—O20A—C26A	118.8 (4)
C112—C105—H10G	107.9	O20A—C26A—C27A	107.2 (5)
C113—C105—H10G	107.9	O20A—C26A—H26A	110.3
O101—C106—C107	107.2 (3)	C27A—C26A—H26A	110.3
O101—C106—H10H	110.3	O20A—C26A—H26B	110.3
C107—C106—H10H	110.3	C27A—C26A—H26B	110.3
O101—C106—H10I	110.3	H26A—C26A—H26B	108.5
C107—C106—H10I	110.3	C26A—C27A—H27A	109.5
H10H—C106—H10I	108.5	C26A—C27A—H27B	109.5
C106—C107—H10J	109.5	H27A—C27A—H27B	109.5
C106—C107—H10K	109.5	C26A—C27A—H27C	109.5
H10J—C107—H10K	109.5	H27A—C27A—H27C	109.5
C106—C107—H10L	109.5	H27B—C27A—H27C	109.5
H10J—C107—H10L	109.5	C201—O20B—C26B	114.2 (4)
H10K—C107—H10L	109.5	O20B—C26B—C27B	108.2 (6)
C110—C108—C103	112.6 (2)	O20B—C26B—H26C	110.1
C110—C108—C109	111.8 (2)	C27B—C26B—H26C	110.1
C103—C108—C109	110.2 (2)	O20B—C26B—H26D	110.1
C110—C108—H10M	107.3	C27B—C26B—H26D	110.1
C103—C108—H10M	107.3	H26C—C26B—H26D	108.4
C109—C108—H10M	107.3	C26B—C27B—H27D	109.5
C108—C109—H10N	109.5	C26B—C27B—H27E	109.5
C108—C109—H10O	109.5	H27D—C27B—H27E	109.5
H10N—C109—H10O	109.5	C26B—C27B—H27F	109.5
C108—C109—H10P	109.5	H27D—C27B—H27F	109.5
H10N—C109—H10P	109.5	H27E—C27B—H27F	109.5
H10O—C109—H10P	109.5		

C6—O1—C1—O2	1.4 (4)	C102—C103—C108—C109	57.2 (3)
C6—O1—C1—C2	−179.9 (2)	C103—C108—C110—C111	−63.2 (3)
O2—C1—C2—O3	−179.1 (2)	C109—C108—C110—C111	61.6 (3)
O1—C1—C2—O3	2.1 (3)	N101—C105—C113—C118	−39.3 (4)
O2—C1—C2—C3	51.8 (3)	C112—C105—C113—C118	83.6 (4)
O1—C1—C2—C3	−126.9 (2)	N101—C105—C113—C114	145.0 (3)
O3—C2—C3—C4	−73.8 (3)	C112—C105—C113—C114	−92.0 (4)
C1—C2—C3—C4	56.0 (3)	C118—C113—C114—C115	0.0 (6)
O3—C2—C3—C8	49.3 (3)	C105—C113—C114—C115	175.8 (3)
C1—C2—C3—C8	179.2 (2)	C113—C114—C115—C116	0.4 (7)
C5—N1—C4—O4	−0.5 (4)	C114—C115—C116—C117	−0.7 (7)
C5—N1—C4—C3	179.1 (2)	C115—C116—C117—C118	0.5 (7)
C8—C3—C4—O4	−58.1 (3)	C114—C113—C118—C117	−0.2 (6)
C2—C3—C4—O4	64.7 (3)	C105—C113—C118—C117	−175.8 (4)
C8—C3—C4—N1	122.2 (2)	C116—C117—C118—C113	0.0 (7)

C2—C3—C4—N1	−115.0 (2)	O202—C201—C202—O203	−175.9 (2)
C4—N1—C5—C13	−90.2 (3)	O20A—C201—C202—O203	19.2 (4)
C4—N1—C5—C12	146.4 (2)	O20B—C201—C202—O203	−5.8 (3)
C1—O1—C6—C7	−150.8 (3)	O202—C201—C202—C203	55.7 (3)
C4—C3—C8—C9	178.0 (3)	O20A—C201—C202—C203	−109.2 (3)
C2—C3—C8—C9	55.4 (3)	O20B—C201—C202—C203	−134.2 (3)
C4—C3—C8—C10	−59.5 (3)	O203—C202—C203—C204	−75.0 (3)
C2—C3—C8—C10	177.9 (2)	C201—C202—C203—C204	54.0 (3)
C9—C8—C10—C11	−66.7 (3)	O203—C202—C203—C208	47.3 (3)
C3—C8—C10—C11	171.1 (2)	C201—C202—C203—C208	176.3 (2)
N1—C5—C13—C18	−39.7 (4)	C205—N201—C204—O204	2.0 (4)
C12—C5—C13—C18	82.7 (3)	C205—N201—C204—C203	−179.0 (2)
N1—C5—C13—C14	143.7 (3)	C208—C203—C204—O204	−51.9 (3)
C12—C5—C13—C14	−93.9 (3)	C202—C203—C204—O204	71.0 (3)
C18—C13—C14—C15	0.6 (5)	C208—C203—C204—N201	129.0 (2)
C5—C13—C14—C15	177.4 (3)	C202—C203—C204—N201	−108.2 (3)
C13—C14—C15—C16	−1.0 (5)	C204—N201—C205—C213	−124.0 (3)
C14—C15—C16—C17	0.3 (5)	C204—N201—C205—C212	111.8 (3)
C15—C16—C17—C18	0.9 (5)	C204—C203—C208—C209	177.5 (2)
C14—C13—C18—C17	0.5 (5)	C202—C203—C208—C209	54.7 (3)
C5—C13—C18—C17	−176.1 (3)	C204—C203—C208—C210	−57.0 (3)
C16—C17—C18—C13	−1.2 (5)	C202—C203—C208—C210	−179.8 (2)
C106—O101—C101—O102	1.1 (4)	C209—C208—C210—C211	57.6 (3)
C106—O101—C101—C102	179.2 (2)	C203—C208—C210—C211	−67.8 (3)
O102—C101—C102—O103	−176.5 (2)	N201—C205—C213—C218	−19.0 (4)
O101—C101—C102—O103	5.4 (3)	C212—C205—C213—C218	104.3 (3)
O102—C101—C102—C103	55.0 (3)	N201—C205—C213—C214	163.8 (3)
O101—C101—C102—C103	−123.1 (2)	C212—C205—C213—C214	−73.0 (4)
O103—C102—C103—C104	−73.8 (3)	C218—C213—C214—C215	0.5 (5)
C101—C102—C103—C104	55.1 (3)	C205—C213—C214—C215	177.8 (3)
O103—C102—C103—C108	50.2 (3)	C213—C214—C215—C216	−0.9 (5)
C101—C102—C103—C108	179.1 (2)	C214—C215—C216—C217	0.5 (5)
C105—N101—C104—O104	1.5 (4)	C215—C216—C217—C218	0.4 (5)
C105—N101—C104—C103	−179.7 (2)	C214—C213—C218—C217	0.4 (5)
C108—C103—C104—O104	−57.4 (3)	C205—C213—C218—C217	−176.8 (3)
C102—C103—C104—O104	65.4 (3)	C216—C217—C218—C213	−0.9 (5)
C108—C103—C104—N101	123.8 (2)	O202—C201—O20A—C26A	9.9 (5)
C102—C103—C104—N101	−113.4 (2)	O20B—C201—O20A—C26A	−107.3 (8)
C104—N101—C105—C112	139.2 (3)	C202—C201—O20A—C26A	175.7 (4)
C104—N101—C105—C113	−96.6 (3)	C201—O20A—C26A—C27A	168.9 (4)
C101—O101—C106—C107	−150.6 (3)	O202—C201—O20B—C26B	−10.7 (6)
C104—C103—C108—C110	−53.7 (3)	O20A—C201—O20B—C26B	67.3 (7)
C102—C103—C108—C110	−177.2 (2)	C202—C201—O20B—C26B	179.7 (4)
C104—C103—C108—C109	−179.3 (2)	C201—O20B—C26B—C27B	−101.8 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O4^{i}	0.88	2.10	2.978 (3)	176
O3—H3···O2^{ii}	0.84 (4)	2.02 (4)	2.809 (3)	156 (3)
N101—H10*C*···O104^{i}	0.88	2.10	2.977 (3)	176
O103—H10*D*···O102^{ii}	0.80 (4)	2.08 (4)	2.808 (3)	152 (4)
N201—H20*A*···O204^{ii}	0.88	2.13	3.004 (3)	175
O203—H20*B*···O202^{i}	0.75 (4)	2.09 (4)	2.795 (3)	158 (4)

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