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The oxalate diester of dehydroepiandrosterone

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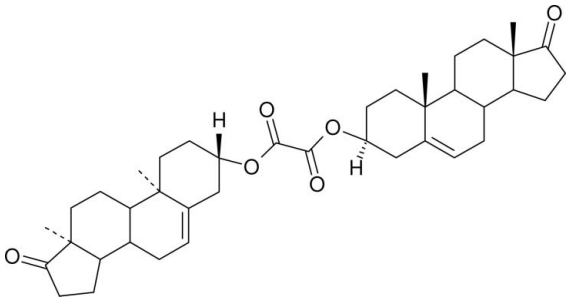
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.101; data-to-parameter ratio = 9.5.

There are two independent molecules of bis(17-oxoandrost-5-en-3β-yl) oxalate, [or bis(DHEA) oxalate], $C_{40}H_{54}O_6$, in the asymmetric unit of the title compound. Molecules are held together by C—H···O hydrogen bonding. There is distortion in the central oxalate section of the molecules and a short intermolecular H···H contact of 2.14 Å is present.

Related literature

For related literature, see: Caira *et al.* (1995); Coppens *et al.* (1969); Cox *et al.* (1990); Nahar *et al.* (2006); Stahly *et al.* (2006); Védova *et al.* (2004).



Experimental

Crystal data

$C_{40}H_{54}O_6$
M_r = 630.83
Monoclinic, $P2_1$
a = 10.9843 (2) Å
b = 22.8189 (4) Å
c = 13.5307 (3) Å
β = 90.4679 (8)°
V = 3391.35 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 120 (2) K
0.4 × 0.18 × 0.12 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.767, T_{max} = 0.990
47104 measured reflections
7977 independent reflections
6961 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.101
S = 1.08
7977 reflections
837 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···O3^{i}	0.99	2.55	3.526 (3)	171
C21—H21A···O12^{ii}	0.99	2.36	3.349 (3)	173
C34—H34···O2^{i}	1.00	2.32	3.239 (3)	152
C47—H47A···O14^{iii}	0.99	2.54	3.439 (3)	151
C62—H62B···O14	0.99	2.56	3.095 (3)	114
C64—H64A···O16^{iii}	0.99	2.57	3.484 (4)	154

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

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2029).

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supplementary materials

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The oxalate diester of dehydroepiandrosterone

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Comment

Crystal structures of DHEA forms have been published (Cox *et al.*, 1990; Caira *et al.*, 1995; Stahly *et al.*, 2006) and details of the importance, uses, preparation and spectroscopic data of the title compound and related symmetrical steroidal dimers are available (Nahar *et al.*, 2006). The atomic arrangement in the molecules of (I) are shown in Figures 1 & 2. There are no classical hydrogen bonds but weak C—H···O contacts hold the molecules together (Table 1). A short H61A···H7A^{i} contact of 2.14Å is also present where C61···C7^{i}=4.019 (4)Å and i indicates coordinates transformed by −1 + *x*, *y*, *z*. The length of the central C*sp*^{2}—C*sp*^{2} bond appears to be different in the two independent molecules with C20—C40=1.542 (4)Å and C60—C80=1.521 (3) Å, but the difference is similar to the accuracy limitation for light atoms caused by the spherical-atom scattering factor approximation (Coppens *et al.*, 1969). Long C*sp*^{2}—C*sp*^{2} bonds are also present in perfluoromethyloxalate (Védova *et al.*, 2004). The oxalate portions of the molecules deviate from planarity, as can be seen by the torsion angles. One oxalate moiety is considerably more non-planar than the other but the overall lengths of the molecules are similar (O3···O6=24.895 (3)Å and O13···O16=24.310 (3) Å). Differences in torsion angles are also evident in the two independent molecules, for example, the C13—C17 ring may be described as a C14 envelope whereas the C53—C57 ring conformation is twisted on C53—C54. The A, B and C ring conformations are chair, half-chair and chair, respectively.

Experimental

Details of the synthesis of (I) have have been published previously (Nahar *et al.*, 2006).

Refinement

All non-hydrogen atoms were refined by full-matrix least squares calculations with anisotropic displacement parameters. All the hydrogen atoms were allowed to ride on their attached atoms with isotropic displacement parameters 1.2 (non-methyl) or 1.3 (methyl) times those of the U_{eq} of their attached atoms. The constrained distances C—H distances were 0.95—1.00 Å.

Figures

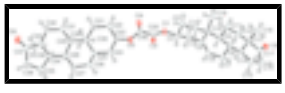


Fig. 1. View of molecule A (50% probability displacement ellipsoids)

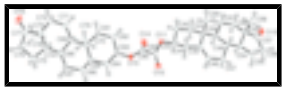


Fig. 2. View of molecule B (50% probability displacement ellipsoids)

Bis(17-oxoandrost-5-en-3β-yl) oxalate

Crystal data

$C_{40}H_{54}O_6$	F_{000} = 1368
M_r = 630.83	D_x = 1.236 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 7932 reflections
a = 10.9843 (2) Å	θ = 2.9–27.5º
b = 22.8189 (4) Å	μ = 0.08 mm^{-1}
c = 13.5307 (3) Å	T = 120 (2) K
β = 90.4679 (8)º	Shard, colourless
V = 3391.35 (11) Å^3	0.4 × 0.18 × 0.12 mm
Z = 4	

Data collection

Bruker Nonius KappaCCD area-detector diffractometer	7977 independent reflections
Radiation source: Bruker Nonius FR591 rotating anode	6961 reflections with $I > 2\sigma(I)$
Monochromator: 10cm confocal mirrors	R_{int} = 0.052
Detector resolution: 9.091 pixels mm^{-1}	θ_{max} = 27.5º
T = 120(2) K	θ_{min} = 3.0º
φ and ω scans to fill Ewald sphere	h = −14→14
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	k = −26→29
T_{min} = 0.767, T_{max} = 0.990	l = −17→17
47104 measured reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 1.0704P]$ where $P = (F_o^2 + 2F_c^2)/3$
Least-squares matrix: full	$(\Delta/\sigma)_{max}$ = 0.001
$R[F^2 > 2\sigma(F^2)]$ = 0.041	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$wR(F^2)$ = 0.101	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
S = 1.08	Extinction correction: none
7977 reflections	
837 parameters	
1 restraint	
H-atom parameters constrained	

Special details

Experimental. Please note cell_measurement_ fields are not relevant to area detector data, the entire data set is used to refine the cell, which is indexed from all observed reflections in a 10 degree phi range.

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.27654 (16)	0.39110 (9)	0.36696 (13)	0.0268 (6)
O2	0.28360 (18)	0.43998 (10)	0.51126 (14)	0.0362 (7)
O3	1.19833 (17)	0.51255 (11)	0.12127 (16)	0.0386 (7)
O4	0.05853 (17)	0.34398 (9)	0.43152 (14)	0.0327 (6)
O5	0.04748 (16)	0.42369 (9)	0.53081 (14)	0.0296 (6)
O6	−0.86836 (18)	0.37757 (10)	0.82784 (16)	0.0406 (7)
C1	0.6213 (2)	0.40740 (14)	0.35944 (19)	0.0294 (8)
C2	0.4984 (2)	0.38118 (14)	0.3902 (2)	0.0316 (9)
C3	0.3967 (2)	0.41569 (13)	0.34180 (19)	0.0251 (8)
C4	0.4067 (2)	0.41395 (14)	0.23054 (18)	0.0262 (8)
C5	0.5293 (2)	0.43738 (12)	0.19843 (17)	0.0221 (7)
C6	0.5344 (2)	0.48089 (13)	0.13302 (19)	0.0257 (8)
C7	0.6504 (2)	0.50557 (13)	0.0928 (2)	0.0271 (8)
C8	0.7619 (2)	0.46846 (12)	0.11729 (18)	0.0219 (7)
C9	0.7578 (2)	0.44600 (12)	0.22445 (18)	0.0225 (7)
C10	0.6417 (2)	0.40917 (12)	0.24610 (19)	0.0229 (7)
C11	0.8770 (2)	0.41332 (15)	0.2528 (2)	0.0318 (9)
C12	0.9939 (2)	0.44914 (15)	0.2334 (2)	0.0337 (9)
C13	0.9951 (2)	0.46925 (13)	0.12583 (19)	0.0254 (8)
C14	0.8782 (2)	0.50416 (12)	0.10579 (18)	0.0238 (7)
C15	0.9032 (3)	0.53751 (14)	0.0095 (2)	0.0305 (8)
C16	1.0359 (3)	0.55726 (14)	0.0245 (2)	0.0346 (9)
C17	1.0928 (2)	0.51328 (14)	0.0959 (2)	0.0292 (8)
C18	1.0131 (3)	0.41725 (13)	0.0542 (2)	0.0335 (9)
C19	0.6546 (3)	0.34619 (13)	0.2067 (2)	0.0347 (9)
C20	0.2320 (2)	0.40929 (13)	0.45218 (19)	0.0256 (8)
C21	−0.2313 (2)	0.36090 (12)	0.6565 (2)	0.0261 (8)
C22	−0.0959 (2)	0.36558 (13)	0.6295 (2)	0.0278 (8)
C23	−0.0816 (2)	0.41334 (13)	0.5541 (2)	0.0265 (8)
C24	−0.1270 (2)	0.47188 (13)	0.5924 (2)	0.0286 (8)
C25	−0.2568 (2)	0.46788 (12)	0.63014 (19)	0.0243 (8)
C26	−0.3393 (2)	0.50685 (12)	0.6018 (2)	0.0261 (8)
C27	−0.4682 (2)	0.50860 (13)	0.6363 (2)	0.0269 (8)
C28	−0.4901 (2)	0.46943 (12)	0.72601 (19)	0.0228 (7)
C29	−0.4245 (2)	0.41036 (12)	0.71200 (18)	0.0210 (7)
C30	−0.2845 (2)	0.41768 (12)	0.70134 (18)	0.0220 (7)

C31	−0.4610 (2)	0.36478 (13)	0.7901 (2)	0.0272 (8)
C32	−0.6000 (2)	0.35675 (13)	0.7984 (2)	0.0270 (8)
C33	−0.6596 (2)	0.41564 (13)	0.82002 (19)	0.0250 (8)
C34	−0.6263 (2)	0.45853 (12)	0.73764 (19)	0.0239 (8)
C35	−0.7150 (2)	0.50985 (14)	0.7496 (2)	0.0312 (8)
C36	−0.8352 (3)	0.47724 (15)	0.7706 (2)	0.0363 (9)
C37	−0.7986 (2)	0.41702 (14)	0.8101 (2)	0.0302 (9)
C38	−0.6304 (3)	0.43788 (14)	0.9247 (2)	0.0320 (9)
C39	−0.2229 (2)	0.43014 (14)	0.8021 (2)	0.0310 (9)
C40	0.1011 (2)	0.38720 (13)	0.46887 (19)	0.0252 (8)
O11	0.19740 (15)	0.69236 (9)	0.04788 (13)	0.0263 (6)
O12	0.23972 (17)	0.75414 (10)	0.17391 (15)	0.0359 (7)
O13	1.09475 (18)	0.63291 (10)	−0.28203 (18)	0.0439 (8)
O14	−0.02565 (18)	0.75112 (11)	0.04883 (15)	0.0406 (7)
O15	−0.01064 (15)	0.73075 (9)	0.21241 (13)	0.0281 (6)
O16	−0.95965 (19)	0.62030 (11)	0.37227 (19)	0.0471 (8)
C41	0.4750 (2)	0.62355 (12)	−0.0640 (2)	0.0252 (8)
C42	0.3415 (2)	0.63001 (12)	−0.0320 (2)	0.0266 (8)
C43	0.3277 (2)	0.68548 (12)	0.02691 (19)	0.0237 (7)
C44	0.3685 (2)	0.73865 (12)	−0.03119 (19)	0.0248 (8)
C45	0.4977 (2)	0.73165 (12)	−0.06773 (18)	0.0228 (7)
C46	0.5797 (2)	0.77333 (12)	−0.04915 (19)	0.0242 (8)
C47	0.7093 (2)	0.77187 (12)	−0.08359 (19)	0.0241 (8)
C48	0.7275 (2)	0.72659 (12)	−0.16549 (18)	0.0214 (7)
C49	0.6651 (2)	0.66863 (12)	−0.13677 (19)	0.0224 (7)
C50	0.5245 (2)	0.67575 (12)	−0.12449 (18)	0.0215 (7)
C51	0.6985 (2)	0.61734 (12)	−0.2063 (2)	0.0281 (8)
C52	0.8356 (2)	0.61090 (13)	−0.2273 (2)	0.0286 (8)
C53	0.8873 (2)	0.66922 (12)	−0.26098 (19)	0.0241 (7)
C54	0.8622 (2)	0.71563 (12)	−0.18203 (19)	0.0240 (8)
C55	0.9464 (3)	0.76702 (13)	−0.2082 (2)	0.0300 (8)
C56	1.0632 (3)	0.73580 (15)	−0.2404 (2)	0.0368 (10)
C57	1.0258 (2)	0.67288 (14)	−0.2651 (2)	0.0307 (9)
C58	0.8387 (2)	0.68677 (14)	−0.3647 (2)	0.0314 (9)
C59	0.4586 (2)	0.67877 (13)	−0.22588 (19)	0.0278 (8)
C60	0.1690 (2)	0.72963 (13)	0.11932 (19)	0.0264 (8)
C61	−0.3297 (2)	0.67005 (14)	0.1980 (2)	0.0312 (8)
C62	−0.1938 (2)	0.67426 (14)	0.1777 (2)	0.0320 (9)
C63	−0.1444 (2)	0.73038 (13)	0.22232 (19)	0.0257 (8)
C64	−0.1688 (2)	0.73280 (14)	0.33261 (19)	0.0272 (8)
C65	−0.3019 (2)	0.72253 (12)	0.35682 (18)	0.0240 (7)
C66	−0.3611 (2)	0.75799 (12)	0.41736 (19)	0.0261 (8)
C67	−0.4915 (2)	0.75037 (13)	0.4470 (2)	0.0280 (8)
C68	−0.5435 (2)	0.69030 (12)	0.42259 (19)	0.0249 (8)
C69	−0.5019 (2)	0.67017 (12)	0.31928 (19)	0.0255 (8)
C70	−0.3602 (2)	0.66861 (12)	0.3090 (2)	0.0256 (8)
C71	−0.5620 (3)	0.61208 (14)	0.2879 (3)	0.0374 (10)
C72	−0.7024 (3)	0.61239 (14)	0.2949 (3)	0.0368 (10)
C73	−0.7400 (2)	0.63190 (13)	0.3974 (2)	0.0316 (9)

C74	−0.6822 (2)	0.69156 (12)	0.42096 (19)	0.0258 (8)
C75	−0.7538 (2)	0.71445 (15)	0.5105 (2)	0.0358 (10)
C76	−0.8856 (3)	0.69720 (17)	0.4813 (2)	0.0416 (10)
C77	−0.8744 (3)	0.64574 (14)	0.4109 (2)	0.0347 (9)
C78	−0.7139 (3)	0.58473 (16)	0.4764 (3)	0.0509 (13)
C79	−0.3063 (3)	0.61348 (13)	0.3583 (3)	0.0369 (10)
C80	0.0318 (2)	0.73837 (13)	0.12178 (19)	0.0271 (8)
H1A	0.68742	0.38414	0.39038	0.0353*
H1B	0.62711	0.44781	0.38567	0.0353*
H2A	0.49372	0.33964	0.36940	0.0379*
H2B	0.49040	0.38283	0.46294	0.0379*
H3	0.40091	0.45733	0.36462	0.0302*
H4A	0.34093	0.43789	0.20055	0.0314*
H4B	0.39688	0.37311	0.20712	0.0314*
H6	0.45980	0.49733	0.11038	0.0308*
H7A	0.66259	0.54544	0.11998	0.0326*
H7B	0.64255	0.50908	0.02014	0.0326*
H8	0.76449	0.43417	0.07132	0.0262*
H9	0.75372	0.48143	0.26779	0.0270*
H11A	0.87424	0.40302	0.32387	0.0381*
H11B	0.88096	0.37630	0.21484	0.0381*
H12A	0.99660	0.48365	0.27773	0.0404*
H12B	1.06648	0.42468	0.24736	0.0404*
H14	0.87527	0.53475	0.15864	0.0286*
H15A	0.84792	0.57149	0.00176	0.0366*
H15B	0.89465	0.51160	−0.04884	0.0366*
H16A	1.07967	0.55719	−0.03914	0.0415*
H16B	1.03900	0.59728	0.05268	0.0415*
H18A	1.01604	0.43187	−0.01387	0.0435*
H18B	0.94501	0.38978	0.06067	0.0435*
H18C	1.08951	0.39714	0.07029	0.0435*
H19A	0.57547	0.32646	0.20888	0.0451*
H19B	0.71341	0.32469	0.24774	0.0451*
H19C	0.68333	0.34734	0.13831	0.0451*
H21A	−0.24138	0.32857	0.70457	0.0313*
H21B	−0.27852	0.35069	0.59636	0.0313*
H22A	−0.04678	0.37474	0.68918	0.0333*
H22B	−0.06704	0.32786	0.60213	0.0333*
H23	−0.12713	0.40266	0.49238	0.0318*
H24A	−0.12359	0.50121	0.53853	0.0342*
H24B	−0.07282	0.48541	0.64653	0.0342*
H26	−0.31460	0.53599	0.55601	0.0313*
H27A	−0.52256	0.49598	0.58160	0.0323*
H27B	−0.48965	0.54947	0.65342	0.0323*
H28	−0.45766	0.48918	0.78672	0.0275*
H29	−0.45425	0.39456	0.64722	0.0252*
H31A	−0.42794	0.37703	0.85518	0.0326*
H31B	−0.42364	0.32663	0.77313	0.0326*
H32A	−0.63298	0.34059	0.73579	0.0324*

H32B	−0.61833	0.32874	0.85213	0.0324*
H34	−0.65222	0.43867	0.67503	0.0287*
H35A	−0.72092	0.53356	0.68848	0.0374*
H35B	−0.69103	0.53547	0.80552	0.0374*
H36A	−0.88370	0.49876	0.82014	0.0435*
H36B	−0.88430	0.47325	0.70928	0.0435*
H38A	−0.65935	0.40937	0.97334	0.0416*
H38B	−0.67106	0.47557	0.93535	0.0416*
H38C	−0.54223	0.44290	0.93226	0.0416*
H39A	−0.13740	0.44055	0.79184	0.0403*
H39B	−0.22754	0.39508	0.84373	0.0403*
H39C	−0.26476	0.46269	0.83466	0.0403*
H41A	0.48280	0.58743	−0.10395	0.0302*
H41B	0.52646	0.61866	−0.00410	0.0302*
H42A	0.28775	0.63139	−0.09108	0.0320*
H42B	0.31746	0.59588	0.00860	0.0320*
H43	0.37511	0.68255	0.09013	0.0285*
H44A	0.31303	0.74449	−0.08840	0.0297*
H44B	0.36354	0.77388	0.01130	0.0297*
H46	0.55440	0.80625	−0.01154	0.0291*
H47A	0.76348	0.76230	−0.02701	0.0289*
H47B	0.73232	0.81112	−0.10840	0.0289*
H48	0.68993	0.74162	−0.22811	0.0257*
H49	0.69800	0.65795	−0.07004	0.0269*
H51A	0.66887	0.58037	−0.17674	0.0337*
H51B	0.65488	0.62282	−0.26999	0.0337*
H52A	0.87864	0.59775	−0.16671	0.0344*
H52B	0.84800	0.58101	−0.27931	0.0344*
H54	0.89449	0.69916	−0.11855	0.0288*
H55A	0.91161	0.79092	−0.26254	0.0360*
H55B	0.96151	0.79246	−0.15008	0.0360*
H56A	1.09820	0.75524	−0.29914	0.0441*
H56B	1.12460	0.73626	−0.18646	0.0441*
H58A	0.85968	0.65623	−0.41258	0.0408*
H58B	0.87567	0.72397	−0.38472	0.0408*
H58C	0.75003	0.69121	−0.36245	0.0408*
H59A	0.37467	0.69206	−0.21656	0.0362*
H59B	0.45819	0.63982	−0.25636	0.0362*
H59C	0.50134	0.70636	−0.26894	0.0362*
H61A	−0.36212	0.63411	0.16639	0.0374*
H61B	−0.37125	0.70405	0.16727	0.0374*
H62A	−0.15111	0.64013	0.20703	0.0384*
H62B	−0.17963	0.67403	0.10555	0.0384*
H63	−0.18089	0.76522	0.18840	0.0308*
H64A	−0.11858	0.70274	0.36643	0.0327*
H64B	−0.14382	0.77164	0.35830	0.0327*
H66	−0.31794	0.79054	0.44384	0.0313*
H67A	−0.54136	0.78060	0.41331	0.0336*
H67B	−0.49791	0.75701	0.51909	0.0336*

H68	−0.51489	0.66139	0.47323	0.0299*
H69	−0.53186	0.70050	0.27159	0.0306*
H71A	−0.52958	0.58021	0.33020	0.0449*
H71B	−0.53890	0.60331	0.21888	0.0449*
H72A	−0.73696	0.63942	0.24478	0.0442*
H72B	−0.73444	0.57259	0.28151	0.0442*
H74	−0.70532	0.71774	0.36458	0.0309*
H75A	−0.74516	0.75741	0.51805	0.0430*
H75B	−0.72764	0.69494	0.57251	0.0430*
H76A	−0.93245	0.68586	0.54046	0.0498*
H76B	−0.92751	0.73041	0.44843	0.0498*
H78A	−0.62672	0.57548	0.47712	0.0659*
H78B	−0.76052	0.54927	0.46083	0.0659*
H78C	−0.73771	0.59949	0.54143	0.0659*
H79A	−0.21727	0.61624	0.35926	0.0480*
H79B	−0.33120	0.57868	0.32079	0.0480*
H79C	−0.33617	0.61044	0.42613	0.0480*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0197 (9)	0.0364 (11)	0.0244 (9)	−0.0019 (8)	0.0038 (7)	−0.0033 (8)
O2	0.0299 (10)	0.0544 (14)	0.0244 (10)	−0.0097 (10)	0.0017 (8)	−0.0066 (10)
O3	0.0220 (10)	0.0502 (13)	0.0435 (12)	−0.0050 (10)	0.0004 (8)	0.0017 (11)
O4	0.0283 (10)	0.0373 (12)	0.0325 (10)	−0.0045 (9)	0.0070 (8)	−0.0079 (9)
O5	0.0213 (9)	0.0330 (11)	0.0346 (10)	−0.0022 (8)	0.0063 (7)	−0.0072 (9)
O6	0.0275 (11)	0.0478 (14)	0.0466 (13)	−0.0087 (10)	0.0064 (9)	−0.0022 (11)
C1	0.0220 (13)	0.0395 (16)	0.0267 (13)	0.0033 (12)	0.0003 (10)	0.0087 (12)
C2	0.0242 (14)	0.0409 (17)	0.0296 (14)	−0.0009 (12)	0.0028 (11)	0.0080 (13)
C3	0.0189 (12)	0.0326 (15)	0.0239 (12)	−0.0028 (11)	0.0018 (9)	0.0005 (11)
C4	0.0196 (12)	0.0370 (16)	0.0220 (12)	0.0013 (11)	0.0007 (9)	−0.0013 (11)
C5	0.0197 (12)	0.0269 (14)	0.0198 (12)	0.0018 (10)	−0.0005 (9)	−0.0061 (10)
C6	0.0202 (12)	0.0330 (15)	0.0238 (13)	0.0060 (11)	−0.0025 (10)	−0.0024 (11)
C7	0.0250 (13)	0.0285 (15)	0.0278 (13)	0.0023 (12)	−0.0032 (10)	0.0044 (12)
C8	0.0203 (12)	0.0232 (13)	0.0221 (12)	−0.0003 (10)	0.0000 (9)	−0.0006 (10)
C9	0.0166 (11)	0.0281 (14)	0.0229 (12)	0.0026 (10)	0.0002 (9)	−0.0027 (11)
C10	0.0196 (12)	0.0248 (14)	0.0244 (12)	0.0026 (10)	0.0013 (9)	0.0004 (11)
C11	0.0202 (12)	0.0437 (18)	0.0314 (14)	0.0030 (12)	0.0027 (10)	0.0148 (13)
C12	0.0209 (13)	0.0488 (19)	0.0313 (15)	0.0019 (13)	0.0013 (11)	0.0088 (13)
C13	0.0192 (12)	0.0293 (14)	0.0277 (13)	−0.0015 (11)	0.0021 (10)	0.0006 (12)
C14	0.0236 (12)	0.0251 (14)	0.0228 (12)	−0.0019 (11)	0.0000 (10)	−0.0006 (11)
C15	0.0284 (14)	0.0314 (15)	0.0316 (15)	−0.0022 (12)	−0.0003 (11)	0.0077 (12)
C16	0.0290 (15)	0.0353 (16)	0.0396 (16)	−0.0100 (13)	0.0022 (12)	0.0049 (13)
C17	0.0253 (13)	0.0342 (16)	0.0280 (14)	−0.0023 (12)	0.0036 (10)	−0.0048 (12)
C18	0.0299 (14)	0.0283 (16)	0.0423 (16)	0.0024 (12)	0.0095 (12)	−0.0015 (13)
C19	0.0282 (14)	0.0264 (15)	0.0497 (18)	0.0010 (12)	0.0081 (13)	−0.0022 (14)
C20	0.0234 (12)	0.0313 (15)	0.0221 (12)	0.0017 (12)	0.0006 (10)	0.0017 (11)
C21	0.0264 (13)	0.0257 (14)	0.0262 (13)	0.0011 (11)	0.0057 (10)	−0.0008 (11)

C22	0.0252 (13)	0.0289 (15)	0.0293 (14)	0.0056 (11)	0.0049 (10)	−0.0046 (11)
C23	0.0181 (12)	0.0327 (15)	0.0289 (14)	−0.0018 (11)	0.0052 (10)	−0.0048 (12)
C24	0.0229 (13)	0.0270 (15)	0.0358 (15)	−0.0023 (11)	0.0037 (11)	−0.0009 (12)
C25	0.0224 (12)	0.0261 (14)	0.0245 (13)	−0.0013 (11)	0.0019 (10)	−0.0046 (11)
C26	0.0250 (13)	0.0227 (14)	0.0307 (14)	−0.0006 (11)	0.0011 (10)	0.0038 (12)
C27	0.0217 (12)	0.0261 (14)	0.0329 (14)	0.0033 (11)	−0.0007 (10)	0.0006 (12)
C28	0.0183 (12)	0.0250 (14)	0.0252 (12)	0.0022 (10)	−0.0011 (9)	−0.0017 (11)
C29	0.0198 (12)	0.0238 (13)	0.0193 (11)	0.0000 (10)	−0.0010 (9)	−0.0016 (10)
C30	0.0188 (12)	0.0240 (14)	0.0231 (12)	0.0019 (10)	−0.0008 (9)	−0.0006 (10)
C31	0.0257 (13)	0.0284 (15)	0.0275 (13)	0.0031 (11)	0.0049 (10)	0.0016 (11)
C32	0.0261 (13)	0.0310 (15)	0.0240 (13)	−0.0030 (12)	0.0041 (10)	−0.0002 (11)
C33	0.0213 (12)	0.0310 (15)	0.0227 (12)	−0.0014 (11)	−0.0003 (9)	−0.0044 (11)
C34	0.0194 (12)	0.0290 (15)	0.0233 (12)	0.0013 (11)	−0.0014 (9)	−0.0037 (11)
C35	0.0246 (13)	0.0315 (15)	0.0374 (15)	0.0035 (12)	−0.0008 (11)	−0.0013 (13)
C36	0.0211 (13)	0.0431 (18)	0.0447 (17)	0.0042 (13)	0.0035 (12)	−0.0025 (14)
C37	0.0223 (13)	0.0395 (17)	0.0288 (14)	−0.0004 (12)	0.0056 (10)	−0.0068 (12)
C38	0.0286 (14)	0.0404 (17)	0.0271 (14)	0.0002 (13)	0.0007 (11)	−0.0059 (13)
C39	0.0221 (13)	0.0448 (18)	0.0262 (13)	0.0026 (12)	−0.0005 (10)	−0.0042 (12)
C40	0.0225 (12)	0.0319 (15)	0.0213 (12)	0.0036 (11)	0.0024 (10)	−0.0007 (11)
O11	0.0170 (8)	0.0324 (11)	0.0297 (10)	−0.0020 (8)	0.0053 (7)	−0.0057 (8)
O12	0.0249 (10)	0.0471 (13)	0.0356 (11)	−0.0023 (9)	0.0026 (8)	−0.0151 (10)
O13	0.0240 (11)	0.0450 (14)	0.0627 (15)	0.0066 (10)	0.0097 (10)	0.0021 (11)
O14	0.0273 (10)	0.0658 (16)	0.0287 (10)	0.0093 (10)	0.0020 (8)	0.0025 (10)
O15	0.0182 (9)	0.0377 (11)	0.0285 (10)	0.0021 (8)	0.0038 (7)	−0.0011 (9)
O16	0.0244 (11)	0.0451 (14)	0.0717 (16)	−0.0029 (10)	−0.0026 (10)	0.0037 (12)
C41	0.0222 (12)	0.0206 (13)	0.0328 (14)	−0.0015 (11)	0.0052 (10)	−0.0004 (11)
C42	0.0207 (12)	0.0251 (14)	0.0342 (15)	−0.0032 (11)	0.0068 (10)	0.0007 (12)
C43	0.0138 (11)	0.0294 (14)	0.0280 (13)	−0.0010 (10)	0.0041 (9)	−0.0008 (11)
C44	0.0220 (12)	0.0261 (14)	0.0263 (13)	0.0007 (11)	0.0026 (10)	−0.0024 (11)
C45	0.0213 (12)	0.0258 (14)	0.0213 (12)	0.0012 (11)	0.0018 (9)	0.0006 (11)
C46	0.0252 (13)	0.0226 (14)	0.0249 (13)	0.0021 (11)	0.0004 (10)	−0.0027 (11)
C47	0.0193 (12)	0.0219 (13)	0.0311 (14)	−0.0026 (10)	−0.0004 (10)	0.0004 (11)
C48	0.0174 (11)	0.0222 (13)	0.0246 (12)	−0.0024 (10)	0.0008 (9)	0.0023 (10)
C49	0.0194 (12)	0.0231 (13)	0.0247 (12)	−0.0001 (10)	0.0027 (9)	0.0002 (10)
C50	0.0188 (11)	0.0218 (13)	0.0240 (12)	−0.0018 (10)	0.0015 (9)	−0.0003 (10)
C51	0.0217 (12)	0.0225 (14)	0.0402 (15)	−0.0036 (11)	0.0099 (11)	−0.0039 (12)
C52	0.0235 (13)	0.0266 (15)	0.0359 (15)	0.0008 (11)	0.0078 (11)	−0.0022 (12)
C53	0.0177 (12)	0.0281 (14)	0.0266 (12)	−0.0010 (11)	0.0029 (9)	0.0002 (11)
C54	0.0197 (12)	0.0282 (15)	0.0242 (13)	−0.0017 (11)	0.0032 (10)	0.0032 (11)
C55	0.0252 (13)	0.0297 (15)	0.0352 (15)	−0.0063 (12)	0.0039 (11)	0.0013 (12)
C56	0.0219 (13)	0.0451 (19)	0.0435 (17)	−0.0101 (13)	0.0072 (12)	−0.0057 (14)
C57	0.0213 (13)	0.0400 (17)	0.0310 (14)	−0.0016 (13)	0.0057 (10)	0.0026 (13)
C58	0.0250 (13)	0.0420 (18)	0.0273 (14)	−0.0014 (13)	0.0031 (10)	−0.0007 (13)
C59	0.0230 (13)	0.0326 (15)	0.0279 (13)	−0.0005 (12)	0.0013 (10)	−0.0047 (12)
C60	0.0232 (13)	0.0330 (15)	0.0229 (12)	0.0014 (12)	0.0028 (10)	−0.0029 (12)
C61	0.0242 (13)	0.0351 (16)	0.0343 (15)	−0.0017 (12)	0.0043 (11)	−0.0135 (13)
C62	0.0256 (14)	0.0350 (17)	0.0354 (15)	0.0012 (12)	0.0059 (11)	−0.0117 (13)
C63	0.0167 (12)	0.0317 (15)	0.0287 (13)	0.0023 (11)	0.0027 (10)	−0.0042 (12)
C64	0.0187 (12)	0.0350 (16)	0.0280 (13)	0.0007 (11)	0.0012 (10)	−0.0028 (12)

C65	0.0212 (12)	0.0288 (14)	0.0221 (12)	0.0012 (11)	0.0022 (9)	0.0010 (11)
C66	0.0251 (13)	0.0259 (14)	0.0273 (13)	−0.0022 (11)	0.0023 (10)	−0.0020 (11)
C67	0.0243 (13)	0.0332 (16)	0.0265 (13)	0.0014 (12)	0.0057 (10)	−0.0051 (11)
C68	0.0217 (12)	0.0279 (14)	0.0251 (13)	0.0011 (11)	−0.0002 (10)	0.0032 (11)
C69	0.0204 (12)	0.0257 (14)	0.0305 (14)	0.0010 (11)	0.0015 (10)	−0.0036 (11)
C70	0.0180 (12)	0.0259 (14)	0.0328 (14)	0.0023 (11)	0.0037 (10)	−0.0052 (11)
C71	0.0270 (14)	0.0320 (16)	0.0534 (19)	−0.0031 (13)	0.0057 (13)	−0.0102 (14)
C72	0.0245 (14)	0.0333 (17)	0.0527 (19)	−0.0041 (13)	−0.0005 (13)	−0.0069 (14)
C73	0.0196 (13)	0.0318 (16)	0.0433 (17)	−0.0025 (12)	0.0014 (11)	0.0084 (13)
C74	0.0219 (12)	0.0288 (15)	0.0267 (13)	0.0015 (11)	0.0009 (10)	0.0050 (11)
C75	0.0241 (14)	0.050 (2)	0.0335 (15)	0.0008 (13)	0.0073 (11)	0.0024 (14)
C76	0.0250 (14)	0.057 (2)	0.0430 (18)	−0.0021 (15)	0.0081 (12)	−0.0005 (16)
C77	0.0240 (14)	0.0361 (17)	0.0440 (17)	−0.0029 (13)	0.0014 (12)	0.0166 (14)
C78	0.0335 (17)	0.0410 (19)	0.078 (3)	−0.0010 (15)	−0.0039 (16)	0.0278 (19)
C79	0.0264 (14)	0.0273 (16)	0.057 (2)	0.0059 (12)	0.0050 (13)	0.0053 (14)
C80	0.0214 (12)	0.0349 (16)	0.0250 (13)	0.0009 (12)	0.0045 (10)	−0.0039 (12)

Geometric parameters (Å, °)

O1—C3	1.477 (3)	C36—H36B	0.9900
O1—C20	1.323 (3)	C36—H36A	0.9900
O2—C20	1.201 (3)	C38—H38B	0.9800
O3—C17	1.206 (3)	C38—H38C	0.9800
O4—C40	1.201 (3)	C38—H38A	0.9800
O5—C23	1.474 (3)	C39—H39B	0.9800
O5—C40	1.323 (3)	C39—H39C	0.9800
O6—C37	1.208 (4)	C39—H39A	0.9800
O11—C60	1.327 (3)	C41—C42	1.540 (3)
O11—C43	1.470 (3)	C41—C50	1.547 (4)
O12—C60	1.205 (3)	C42—C43	1.504 (4)
O13—C57	1.209 (4)	C43—C44	1.516 (4)
O14—C80	1.203 (3)	C44—C45	1.515 (3)
O15—C80	1.327 (3)	C45—C46	1.332 (4)
O15—C63	1.477 (3)	C45—C50	1.519 (4)
O16—C77	1.216 (4)	C46—C47	1.502 (3)
C1—C2	1.537 (3)	C47—C48	1.529 (4)
C1—C10	1.552 (4)	C48—C49	1.541 (4)
C2—C3	1.512 (4)	C48—C54	1.519 (3)
C3—C4	1.511 (4)	C49—C50	1.563 (3)
C4—C5	1.516 (3)	C49—C51	1.548 (4)
C5—C6	1.332 (4)	C50—C59	1.547 (3)
C5—C10	1.530 (3)	C51—C52	1.542 (3)
C6—C7	1.499 (3)	C52—C53	1.518 (4)
C7—C8	1.523 (3)	C53—C54	1.531 (4)
C8—C14	1.524 (3)	C53—C57	1.525 (3)
C8—C9	1.539 (3)	C53—C58	1.550 (4)
C9—C11	1.552 (3)	C54—C55	1.537 (4)
C9—C10	1.557 (3)	C55—C56	1.534 (5)
C10—C19	1.540 (4)	C56—C57	1.530 (5)

C11—C12	1.546 (4)	C60—C80	1.521 (3)
C12—C13	1.526 (4)	C61—C62	1.523 (3)
C13—C14	1.533 (3)	C61—C70	1.542 (4)
C13—C17	1.527 (4)	C62—C63	1.514 (4)
C13—C18	1.546 (4)	C63—C64	1.519 (4)
C14—C15	1.536 (4)	C64—C65	1.519 (3)
C15—C16	1.538 (5)	C65—C66	1.326 (4)
C16—C17	1.524 (4)	C65—C70	1.528 (4)
C20—C40	1.542 (3)	C66—C67	1.501 (3)
C21—C22	1.538 (3)	C67—C68	1.520 (4)
C21—C30	1.547 (4)	C68—C69	1.544 (4)
C22—C23	1.502 (4)	C68—C74	1.524 (3)
C23—C24	1.519 (4)	C69—C70	1.564 (3)
C24—C25	1.521 (3)	C69—C71	1.539 (4)
C25—C30	1.529 (4)	C70—C79	1.540 (4)
C25—C26	1.324 (4)	C71—C72	1.546 (5)
C26—C27	1.495 (3)	C72—C73	1.517 (5)
C27—C28	1.528 (4)	C73—C74	1.535 (4)
C28—C29	1.541 (4)	C73—C77	1.522 (4)
C28—C34	1.526 (3)	C73—C78	1.542 (5)
C29—C30	1.555 (3)	C74—C75	1.541 (4)
C29—C31	1.538 (4)	C75—C76	1.548 (4)
C30—C39	1.544 (4)	C76—C77	1.518 (5)
C31—C32	1.543 (3)	C41—H41A	0.9900
C32—C33	1.524 (4)	C41—H41B	0.9900
C33—C38	1.536 (4)	C42—H42A	0.9900
C33—C34	1.530 (4)	C42—H42B	0.9900
C33—C37	1.532 (3)	C43—H43	1.0000
C34—C35	1.533 (4)	C44—H44A	0.9900
C35—C36	1.544 (4)	C44—H44B	0.9900
C36—C37	1.527 (5)	C46—H46	0.9500
C1—H1B	0.9900	C47—H47A	0.9900
C1—H1A	0.9900	C47—H47B	0.9900
C2—H2B	0.9900	C48—H48	1.0000
C2—H2A	0.9900	C49—H49	1.0000
C3—H3	1.0000	C51—H51A	0.9900
C4—H4B	0.9900	C51—H51B	0.9900
C4—H4A	0.9900	C52—H52A	0.9900
C6—H6	0.9500	C52—H52B	0.9900
C7—H7A	0.9900	C54—H54	1.0000
C7—H7B	0.9900	C55—H55A	0.9900
C8—H8	1.0000	C55—H55B	0.9900
C9—H9	1.0000	C56—H56A	0.9900
C11—H11A	0.9900	C56—H56B	0.9900
C11—H11B	0.9900	C58—H58A	0.9800
C12—H12A	0.9900	C58—H58B	0.9800
C12—H12B	0.9900	C58—H58C	0.9800
C14—H14	1.0000	C59—H59A	0.9800
C15—H15B	0.9900	C59—H59B	0.9800

C15—H15A	0.9900	C59—H59C	0.9800
C16—H16A	0.9900	C61—H61A	0.9900
C16—H16B	0.9900	C61—H61B	0.9900
C18—H18A	0.9800	C62—H62A	0.9900
C18—H18B	0.9800	C62—H62B	0.9900
C18—H18C	0.9800	C63—H63	1.0000
C19—H19B	0.9800	C64—H64A	0.9900
C19—H19A	0.9800	C64—H64B	0.9900
C19—H19C	0.9800	C66—H66	0.9500
C21—H21B	0.9900	C67—H67A	0.9900
C21—H21A	0.9900	C67—H67B	0.9900
C22—H22B	0.9900	C68—H68	1.0000
C22—H22A	0.9900	C69—H69	1.0000
C23—H23	1.0000	C71—H71A	0.9900
C24—H24B	0.9900	C71—H71B	0.9900
C24—H24A	0.9900	C72—H72A	0.9900
C26—H26	0.9500	C72—H72B	0.9900
C27—H27A	0.9900	C74—H74	1.0000
C27—H27B	0.9900	C75—H75A	0.9900
C28—H28	1.0000	C75—H75B	0.9900
C29—H29	1.0000	C76—H76A	0.9900
C31—H31A	0.9900	C76—H76B	0.9900
C31—H31B	0.9900	C78—H78A	0.9800
C32—H32A	0.9900	C78—H78B	0.9800
C32—H32B	0.9900	C78—H78C	0.9800
C34—H34	1.0000	C79—H79A	0.9800
C35—H35A	0.9900	C79—H79B	0.9800
C35—H35B	0.9900	C79—H79C	0.9800
O1···O4	2.773 (3)	H19C···C11	3.0200
O2···C34^{i}	3.239 (3)	H21A···C31	2.8100
O2···O5	2.636 (3)	H21A···O12^{x}	2.3600
O2···C2	3.180 (3)	H21A···H31B	2.2100
O2···C78^{i}	3.337 (4)	H21A···H39B	2.4200
O4···C22	3.220 (3)	H21B···H29	2.2900
O4···O1	2.773 (3)	H21B···H23	2.4900
O5···O2	2.636 (3)	H21B···H67A^{vii}	2.5500
O11···O14	2.793 (3)	H22A···O6^{i}	2.7000
O12···O15	2.854 (3)	H22A···C39	2.7800
O12···C21^{ii}	3.349 (3)	H22A···H39A	2.2800
O12···C44	3.145 (3)	H22B···C40	2.9200
O14···C62	3.095 (3)	H22B···H76B^{vii}	2.3300
O14···O11	2.793 (3)	H22B···O4	2.7200
O15···O12	2.854 (3)	H23···H11A^{iii}	2.2800
O1···H12B^{iii}	2.9100	H23···O4	2.5800
O2···H78B^{i}	2.6300	H23···H1A^{iii}	2.4900
O2···H2B	2.7000	H23···H21B	2.4900

O2···H27A^{i}	2.6500	H24A···H26	2.2600
O2···H3	2.4100	H24B···H39A	2.3300
O2···H34^{i}	2.3200	H24B···H36B^{i}	2.2500
O3···H42B^{i}	2.7700	H24B···C36^{i}	3.1000
O3···H6^{i}	2.9000	H24B···H52B^{xi}	2.5600
O3···H72B^{iv}	2.6600	H24B···C39	2.9700
O3···H4A^{i}	2.5500	H26···H24A	2.2600
O4···H55A^{v}	2.6100	H26···H79C	2.4500
O4···H11A^{iii}	2.8300	H27A···H29	2.5900
O4···H58B^{v}	2.9000	H27A···H34	2.3200
O4···H22B	2.7200	H27A···H78A	2.5600
O4···H23	2.5800	H27A···O2^{iii}	2.6500
O5···H36B^{i}	2.7600	H27B···H51B^{xi}	2.5200
O6···H18A^{vi}	2.7900	H27B···H59B^{xi}	2.4700
O6···H22A^{iii}	2.7000	H27B···C35	2.9500
O6···H63^{vii}	2.6300	H28···H38C	2.4300
O11···H16B^{iii}	2.7800	H28···H39C	2.2900
O12···H43	2.4900	H28···H51A^{xi}	2.5500
O12···H72A^{i}	2.8000	H28···C38	2.9200
O12···H74^{i}	2.7700	H28···C39	2.9200
O12···H44B	2.6300	H29···H21B	2.2900
O12···H21A^{ii}	2.3600	H29···C26	2.9200
O12···H31B^{ii}	2.7000	H29···H2B^{iii}	2.5800
O13···H76A^{viii}	2.7000	H29···H34	2.4300
O14···H63	2.5700	H29···H27A	2.5900
O14···H55B^{iii}	2.8500	H31A···C38	2.7900
O14···H47A^{iii}	2.5400	H31A···C39	2.6600
O14···H62B	2.5600	H31A···H39B	2.2500
O14···H54^{iii}	2.7000	H31A···H38C	2.2200
O16···H79A^{iii}	2.8400	H31B···C21	2.7600
O16···H64A^{iii}	2.5700	H31B···O12^{x}	2.7000
C2···O2	3.180 (3)	H31B···H21A	2.2100
C6···C38^{ix}	3.479 (4)	H32A···C65^{vii}	3.0500
C19···C44^{v}	3.423 (4)	H32A···H34	2.3900
C21···O12^{x}	3.349 (3)	H32A···C66^{vii}	2.8000
C22···O4	3.220 (3)	H32B···H46^{x}	2.3200
C34···O2^{iii}	3.239 (3)	H32B···H38A	2.5100
C38···C6^{xi}	3.479 (4)	H32B···C46^{x}	2.9800
C44···O12	3.145 (3)	H34···H27A	2.3200
C44···C19^{xii}	3.423 (4)	H34···H29	2.4300
C62···O14	3.095 (3)	H34···O2^{iii}	2.3200
C78···O2^{iii}	3.337 (4)	H34···H32A	2.3900

C1···H11A	2.8300	H35A···H78C	2.5000
C2···H19A	2.8900	H35A···C27	2.9300
C2···H67B^{x}	3.0900	H35A···C78	3.1000
C4···H19A	2.7400	H35B···C38	2.8300
C6···H9	3.0100	H35B···C42^{xi}	3.1000
C6···H38C^{ix}	2.9700	H35B···H38B	2.2400
C7···H15A	2.9200	H35B···H41A^{xi}	2.5500
C8···H18B	2.8100	H36A···H16A^{vi}	2.3600
C8···H19C	2.9100	H36B···H24B^{iii}	2.2500
C11···H19C	3.0200	H36B···O5^{iii}	2.7600
C11···H1A	2.8800	H36B···C24^{iii}	3.0900
C11···H19B	2.7100	H38A···H32B	2.5100
C11···H18B	2.7600	H38B···C35	2.6700
C11···H14	3.0500	H38B···C36	2.8600
C15···H7B	2.9400	H38B···H35B	2.2400
C15···H7A	3.0500	H38C···C31	2.7800
C15···H52A	2.7600	H38C···H31A	2.2200
C15···H18A	2.7300	H38C···C28	2.9200
C16···H18A	2.9200	H38C···H28	2.4300
C18···H15B	2.8700	H38C···C6^{xi}	2.9700
C18···H8	2.7700	H39A···C22	2.8200
C18···H11B	2.7800	H39A···H24B	2.3300
C19···H4B	2.9000	H39A···C24	2.7900
C19···H8	2.9800	H39A···H22A	2.2800
C19···H2A	2.8400	H39B···H31A	2.2500
C19···H11B	2.5800	H39B···H21A	2.4200
C19···H44A^{v}	2.8400	H39B···C31	2.7500
C20···H2B	2.9000	H39C···H15B^{xi}	2.6000
C21···H31B	2.7600	H39C···H28	2.2900
C22···H39A	2.8200	H39C···C28	2.8700
C24···H52B^{xi}	3.0500	H41A···C51	2.8400
C24···H39A	2.7900	H41A···H35B^{ix}	2.5500
C24···H36B^{i}	3.0900	H41A···H51A	2.2800
C25···H52B^{xi}	3.0800	H41A···H59B	2.4000
C26···H29	2.9200	H41B···H43	2.5600
C27···H35A	2.9300	H41B···H49	2.2800
C28···H39C	2.8700	H42A···C59	2.8400
C28···H38C	2.9200	H42A···H44A	2.6000
C31···H21A	2.8100	H42A···H59A	2.4000
C31···H38C	2.7800	H42B···O3^{iii}	2.7700
C31···H39B	2.7500	H43···O12	2.4900
C35···H38B	2.6700	H43···H41B	2.5600
C35···H27B	2.9500	H44A···C59	2.8800
C36···H38B	2.8600	H44A···H42A	2.6000
C36···H24B^{iii}	3.1000	H44A···H56B^{iii}	2.4600

C38···H35B	2.8300	H44A···H59A	2.2200
C38···H31A	2.7900	H44A···C19^{xii}	2.8400
C38···H28	2.9200	H44A···H19C^{xii}	2.4400
C38···H6^{xi}	3.0200	H44B···O12	2.6300
C39···H15B^{xi}	3.0200	H44B···C60	2.7900
C39···H31A	2.6600	H44B···H46	2.2500
C39···H24B	2.9700	H46···H44B	2.2500
C39···H28	2.9200	H46···H32B^{ii}	2.3200
C39···H22A	2.7800	H47A···O14^{i}	2.5400
C40···H22B	2.9200	H47A···H49	2.5500
C41···H51A	2.8100	H47A···H54	2.3900
C42···H35B^{ix}	3.1000	H47B···C55	2.9000
C42···H59A	2.9000	H47B···H4B^{xii}	2.4000
C44···H59A	2.7300	H48···C45	3.0500
C44···H19C^{xii}	2.9300	H48···C58	2.7800
C45···H48	3.0500	H48···C59	2.9200
C45···H19A^{xii}	2.9900	H48···H58C	2.2500
C46···H49	2.9500	H48···H59C	2.2900
C46···H32B^{ii}	2.9800	H49···C46	2.9500
C46···H19A^{xii}	3.0000	H49···H41B	2.2800
C47···H55B	2.9600	H49···H47A	2.5500
C47···H4B^{xii}	3.0800	H49···H54	2.4500
C48···H59C	2.8800	H51A···C41	2.8100
C48···H58C	2.8000	H51A···H28^{ix}	2.5500
C51···H58C	2.7700	H51A···H41A	2.2800
C51···H41A	2.8400	H51B···C58	2.8100
C51···H54	3.0800	H51B···C59	2.5800
C51···H59B	2.7700	H51B···H27B^{ix}	2.5200
C51···H59C	3.0800	H51B···H58C	2.2600
C55···H47B	2.9000	H51B···H59B	2.2000
C55···H58B	2.6900	H51B···H59C	2.5500
C56···H58B	2.8400	H52A···C15	2.7600
C57···H76A^{viii}	2.6900	H52A···H15A	2.3800
C58···H76A^{viii}	2.8300	H52A···H15B	2.5400
C58···H51B	2.8100	H52A···H54	2.4100
C58···H55A	2.8600	H52B···C24^{ix}	3.0500
C58···H48	2.7800	H52B···C25^{ix}	3.0800
C59···H42A	2.8400	H52B···H24B^{ix}	2.5600
C59···H48	2.9200	H52B···H58A	2.4900
C59···H51B	2.5800	H54···O14^{i}	2.7000
C59···H44A	2.8800	H54···C51	3.0800
C60···H72A^{i}	2.8600	H54···H47A	2.3900
C60···H44B	2.7900	H54···H49	2.4500
C61···H7A^{iii}	3.0300	H54···H52A	2.4100

C61···H71B	2.7700	H55A···C58	2.8600
C62···H79A	2.8000	H55A···H58B	2.2800
C64···H79A	2.7400	H55A···O4^{xii}	2.6100
C64···H76B^{i}	3.0700	H55B···O14^{i}	2.8500
C65···H32A^{xiii}	3.0500	H55B···C47	2.9600
C66···H32A^{xiii}	2.8000	H56B···H44A^{i}	2.4600
C66···H69	3.0100	H58A···H52B	2.4900
C67···H75A	2.9600	H58A···H76A^{viii}	2.4700
C68···H78A	2.8700	H58B···C55	2.6900
C68···H79C	2.9200	H58B···C56	2.8400
C71···H79C	3.0900	H58B···H55A	2.2800
C71···H74	3.0700	H58B···H76A^{viii}	2.5000
C71···H61A	2.8000	H58B···O4^{xii}	2.9000
C71···H79B	2.6800	H58C···C48	2.8000
C71···H78A	2.7900	H58C···C51	2.7700
C75···H67B	2.9800	H58C···H48	2.2500
C75···H78C	2.6600	H58C···H51B	2.2600
C75···H67A	3.0800	H59A···C42	2.9000
C76···H78C	2.8700	H59A···C44	2.7300
C76···H64A^{iii}	2.9900	H59A···H42A	2.4000
C77···H64A^{iii}	3.0400	H59A···H44A	2.2200
C78···H35A	3.1000	H59B···C51	2.7700
C78···H68	2.8000	H59B···H27B^{ix}	2.4700
C78···H71A	2.8400	H59B···H41A	2.4000
C78···H75B	2.8400	H59B···H51B	2.2000
C79···H62A	2.7400	H59C···C48	2.8800
C79···H64A	2.9000	H59C···C51	3.0800
C79···H68	2.9900	H59C···H48	2.2900
C79···H71A	2.5900	H59C···H51B	2.5500
C80···H62B	2.7500	H61A···C71	2.8000
H1A···C11	2.8800	H61A···H7A^{iii}	2.1400
H1A···H11A	2.2900	H61A···H71B	2.1900
H1A···H19B	2.3800	H61A···H79B	2.4600
H1A···H23^{i}	2.4900	H61B···H63	2.5300
H1B···H3	2.5100	H61B···H69	2.2700
H1B···H9	2.2600	H62A···C79	2.7400
H2A···C19	2.8400	H62A···H14^{iii}	2.5100
H2A···H67B^{x}	2.4200	H62A···H79A	2.2600
H2A···H19A	2.3800	H62B···O14	2.5600
H2A···H4B	2.5500	H62B···C80	2.7500
H2B···O2	2.7000	H63···O14	2.5700
H2B···H29^{i}	2.5800	H63···H61B	2.5300
H2B···C20	2.9000	H63···O6^{xiii}	2.6300
H3···O2	2.4100	H64A···O16^{i}	2.5700
H3···H1B	2.5100	H64A···C76^{i}	2.9900

H4A···O3^{iii}	2.5500	H64A···C77^{i}	3.0400
H4A···H6	2.2500	H64A···C79	2.9000
H4B···H2A	2.5500	H64A···H76B^{i}	2.4500
H4B···C19	2.9000	H64A···H79A	2.2500
H4B···H47B^{v}	2.4000	H64B···H66	2.2800
H4B···H19A	2.2300	H66···H64B	2.2800
H4B···C47^{v}	3.0800	H67A···C75	3.0800
H6···O3^{iii}	2.9000	H67A···H74	2.3900
H6···C38^{ix}	3.0200	H67A···H21B^{xiii}	2.5500
H6···H4A	2.2500	H67B···C75	2.9800
H7A···C15	3.0500	H67B···C2^{ii}	3.0900
H7A···H61A^{i}	2.1400	H67B···H2A^{ii}	2.4200
H7A···C61^{i}	3.0300	H68···C78	2.8000
H7A···H14	2.4000	H68···C79	2.9900
H7B···C15	2.9400	H68···H78A	2.3100
H8···C19	2.9800	H68···H79C	2.3700
H8···H18B	2.2300	H69···C66	3.0100
H8···H19C	2.3600	H69···H61B	2.2700
H8···C18	2.7700	H69···H74	2.3300
H9···H79B^{i}	2.5100	H71A···C78	2.8400
H9···C6	3.0100	H71A···C79	2.5900
H9···H1B	2.2600	H71A···H78A	2.2700
H9···H14	2.3400	H71A···H79B	2.1800
H11A···O4^{i}	2.8300	H71A···H79C	2.5700
H11A···C1	2.8300	H71B···C61	2.7700
H11A···H1A	2.2900	H71B···H61A	2.1900
H11A···H23^{i}	2.2800	H72A···O12^{iii}	2.8000
H11B···H19C	2.4900	H72A···C60^{iii}	2.8600
H11B···C18	2.7800	H72A···H74	2.4400
H11B···C19	2.5800	H72B···O3^{xiv}	2.6600
H11B···H19B	2.2300	H72B···H78B	2.5000
H11B···H18B	2.2300	H74···O12^{iii}	2.7700
H12A···H14	2.3900	H74···C71	3.0700
H12B···H18C	2.4900	H74···H67A	2.3900
H12B···O1^{i}	2.9100	H74···H69	2.3300
H14···H7A	2.4000	H74···H72A	2.4400
H14···H9	2.3400	H75A···C67	2.9600
H14···H12A	2.3900	H75B···C78	2.8400
H14···H62A^{i}	2.5100	H75B···H78C	2.2200
H14···C11	3.0500	H76A···O13^{vi}	2.7000
H15A···C7	2.9200	H76A···C57^{vi}	2.6900
H15A···H52A	2.3800	H76A···C58^{vi}	2.8300
H15B···H18A	2.3000	H76A···H58A^{vi}	2.4700
H15B···H39C^{ix}	2.6000	H76A···H58B^{vi}	2.5000

H15B···H52A	2.5400	H76B···C64^{iii}	3.0700
H15B···C18	2.8700	H76B···H64A^{iii}	2.4500
H15B···C39^{ix}	3.0200	H76B···H22B^{xiii}	2.3300
H16A···H36A^{viii}	2.3600	H78A···C68	2.8700
H16B···O11^{i}	2.7800	H78A···C71	2.7900
H18A···O6^{viii}	2.7900	H78A···H27A	2.5600
H18A···C16	2.9200	H78A···H68	2.3100
H18A···H15B	2.3000	H78A···H71A	2.2700
H18A···C15	2.7300	H78B···O2^{iii}	2.6300
H18B···C8	2.8100	H78B···H72B	2.5000
H18B···H8	2.2300	H78C···C75	2.6600
H18B···H11B	2.2300	H78C···C76	2.8700
H18B···C11	2.7600	H78C···H35A	2.5000
H18C···H12B	2.4900	H78C···H75B	2.2200
H19A···C45^{v}	2.9900	H79A···O16^{i}	2.8400
H19A···C46^{v}	3.0000	H79A···C62	2.8000
H19A···H4B	2.2300	H79A···C64	2.7400
H19A···C2	2.8900	H79A···H62A	2.2600
H19A···C4	2.7400	H79A···H64A	2.2500
H19A···H2A	2.3800	H79B···C71	2.6800
H19B···H1A	2.3800	H79B···H9^{iii}	2.5100
H19B···H11B	2.2300	H79B···H61A	2.4600
H19B···C11	2.7100	H79B···H71A	2.1800
H19C···H8	2.3600	H79C···C68	2.9200
H19C···H11B	2.4900	H79C···C71	3.0900
H19C···C44^{v}	2.9300	H79C···H26	2.4500
H19C···H44A^{v}	2.4400	H79C···H68	2.3700
H19C···C8	2.9100	H79C···H71A	2.5700
C3—O1—C20	114.8 (2)	H39A—C39—H39B	109.00
C23—O5—C40	117.9 (2)	C30—C39—H39A	109.00
C43—O11—C60	116.38 (19)	C42—C41—C50	114.5 (2)
C63—O15—C80	116.24 (18)	C41—C42—C43	109.3 (2)
C2—C1—C10	114.3 (2)	O11—C43—C42	107.14 (19)
C1—C2—C3	109.1 (2)	O11—C43—C44	107.9 (2)
O1—C3—C4	106.99 (19)	C42—C43—C44	111.6 (2)
O1—C3—C2	111.2 (2)	C43—C44—C45	111.5 (2)
C2—C3—C4	111.0 (2)	C44—C45—C46	119.8 (2)
C3—C4—C5	110.39 (19)	C44—C45—C50	116.1 (2)
C4—C5—C10	116.5 (2)	C46—C45—C50	124.2 (2)
C4—C5—C6	119.7 (2)	C45—C46—C47	124.5 (2)
C6—C5—C10	123.8 (2)	C46—C47—C48	111.7 (2)
C5—C6—C7	124.2 (2)	C47—C48—C49	109.6 (2)
C6—C7—C8	113.4 (2)	C47—C48—C54	110.6 (2)
C9—C8—C14	107.77 (19)	C49—C48—C54	109.4 (2)
C7—C8—C14	110.7 (2)	C48—C49—C50	112.3 (2)
C7—C8—C9	111.1 (2)	C48—C49—C51	112.8 (2)

C8—C9—C11	111.21 (19)	C50—C49—C51	112.5 (2)
C8—C9—C10	112.79 (19)	C41—C50—C45	108.0 (2)
C10—C9—C11	112.6 (2)	C41—C50—C49	109.2 (2)
C1—C10—C9	109.0 (2)	C41—C50—C59	109.9 (2)
C1—C10—C5	107.75 (19)	C45—C50—C49	109.7 (2)
C5—C10—C19	108.8 (2)	C45—C50—C59	108.6 (2)
C9—C10—C19	111.2 (2)	C49—C50—C59	111.46 (19)
C1—C10—C19	109.4 (2)	C49—C51—C52	114.9 (2)
C5—C10—C9	110.7 (2)	C51—C52—C53	109.9 (2)
C9—C11—C12	113.8 (3)	C52—C53—C54	109.1 (2)
C11—C12—C13	109.5 (2)	C52—C53—C57	115.8 (2)
C12—C13—C14	108.1 (2)	C52—C53—C58	111.8 (2)
C14—C13—C17	101.6 (2)	C54—C53—C57	100.0 (2)
C14—C13—C18	113.5 (2)	C54—C53—C58	113.0 (2)
C17—C13—C18	104.2 (2)	C57—C53—C58	106.8 (2)
C12—C13—C18	111.7 (2)	C48—C54—C53	113.5 (2)
C12—C13—C17	117.5 (2)	C48—C54—C55	119.8 (2)
C8—C14—C15	120.5 (2)	C53—C54—C55	104.8 (2)
C8—C14—C13	113.9 (2)	C54—C55—C56	102.6 (2)
C13—C14—C15	104.6 (2)	C55—C56—C57	105.9 (2)
C14—C15—C16	102.1 (2)	O13—C57—C53	126.3 (3)
C15—C16—C17	105.9 (2)	O13—C57—C56	125.6 (2)
C13—C17—C16	108.4 (2)	C53—C57—C56	108.0 (2)
O3—C17—C13	126.2 (3)	O11—C60—O12	126.2 (2)
O3—C17—C16	125.3 (3)	O11—C60—C80	109.8 (2)
O1—C20—O2	125.9 (2)	O12—C60—C80	124.0 (2)
O1—C20—C40	112.2 (2)	C62—C61—C70	113.5 (2)
O2—C20—C40	121.9 (2)	C61—C62—C63	109.3 (2)
C22—C21—C30	113.8 (2)	O15—C63—C62	108.8 (2)
C21—C22—C23	108.6 (2)	O15—C63—C64	105.82 (18)
C22—C23—C24	111.7 (2)	C62—C63—C64	110.9 (2)
O5—C23—C24	104.6 (2)	C63—C64—C65	112.6 (2)
O5—C23—C22	111.6 (2)	C64—C65—C66	121.1 (2)
C23—C24—C25	111.9 (2)	C64—C65—C70	115.7 (2)
C26—C25—C30	123.1 (2)	C66—C65—C70	123.2 (2)
C24—C25—C26	120.2 (2)	C65—C66—C67	124.7 (2)
C24—C25—C30	116.6 (2)	C66—C67—C68	113.8 (2)
C25—C26—C27	125.1 (2)	C67—C68—C69	110.6 (2)
C26—C27—C28	112.8 (2)	C67—C68—C74	111.1 (2)
C27—C28—C34	109.8 (2)	C69—C68—C74	107.2 (2)
C27—C28—C29	109.7 (2)	C68—C69—C70	112.9 (2)
C29—C28—C34	109.3 (2)	C68—C69—C71	112.1 (2)
C28—C29—C31	112.5 (2)	C70—C69—C71	112.4 (2)
C28—C29—C30	112.4 (2)	C61—C70—C65	107.6 (2)
C30—C29—C31	113.6 (2)	C61—C70—C69	108.09 (19)
C21—C30—C39	109.7 (2)	C61—C70—C79	110.7 (2)
C25—C30—C29	109.94 (19)	C65—C70—C69	111.0 (2)
C25—C30—C39	109.3 (2)	C65—C70—C79	108.4 (2)
C29—C30—C39	111.39 (19)	C69—C70—C79	111.1 (2)

C21—C30—C25	107.6 (2)	C69—C71—C72	113.9 (3)
C21—C30—C29	108.9 (2)	C71—C72—C73	109.7 (3)
C29—C31—C32	113.2 (2)	C72—C73—C74	109.6 (2)
C31—C32—C33	109.6 (2)	C72—C73—C77	116.2 (2)
C32—C33—C38	112.4 (2)	C72—C73—C78	112.2 (3)
C34—C33—C37	99.6 (2)	C74—C73—C77	101.0 (2)
C34—C33—C38	114.3 (2)	C74—C73—C78	113.6 (2)
C37—C33—C38	105.9 (2)	C77—C73—C78	103.7 (2)
C32—C33—C34	108.6 (2)	C68—C74—C73	113.5 (2)
C32—C33—C37	115.5 (2)	C68—C74—C75	120.8 (2)
C28—C34—C33	114.8 (2)	C73—C74—C75	104.5 (2)
C33—C34—C35	104.8 (2)	C74—C75—C76	101.3 (2)
C28—C34—C35	120.7 (2)	C75—C76—C77	106.1 (3)
C34—C35—C36	101.3 (2)	O16—C77—C73	126.4 (3)
C35—C36—C37	106.0 (2)	O16—C77—C76	125.0 (3)
O6—C37—C33	126.9 (3)	C73—C77—C76	108.6 (3)
O6—C37—C36	125.1 (2)	O14—C80—O15	127.2 (2)
C33—C37—C36	108.0 (2)	O14—C80—C60	121.8 (2)
O4—C40—O5	127.6 (2)	O15—C80—C60	111.0 (2)
O5—C40—C20	107.9 (2)	C42—C41—H41A	109.00
O4—C40—C20	124.5 (2)	C42—C41—H41B	109.00
C2—C1—H1B	109.00	C50—C41—H41A	109.00
C2—C1—H1A	109.00	C50—C41—H41B	109.00
H1A—C1—H1B	108.00	H41A—C41—H41B	108.00
C10—C1—H1A	109.00	C41—C42—H42A	110.00
C10—C1—H1B	109.00	C41—C42—H42B	110.00
C3—C2—H2A	110.00	C43—C42—H42A	110.00
C3—C2—H2B	110.00	C43—C42—H42B	110.00
H2A—C2—H2B	108.00	H42A—C42—H42B	108.00
C1—C2—H2B	110.00	O11—C43—H43	110.00
C1—C2—H2A	110.00	C42—C43—H43	110.00
C2—C3—H3	109.00	C44—C43—H43	110.00
C4—C3—H3	109.00	C43—C44—H44A	109.00
O1—C3—H3	109.00	C43—C44—H44B	109.00
C5—C4—H4A	110.00	C45—C44—H44A	109.00
C3—C4—H4A	110.00	C45—C44—H44B	109.00
C3—C4—H4B	110.00	H44A—C44—H44B	108.00
H4A—C4—H4B	108.00	C45—C46—H46	118.00
C5—C4—H4B	110.00	C47—C46—H46	118.00
C7—C6—H6	118.00	C46—C47—H47A	109.00
C5—C6—H6	118.00	C46—C47—H47B	109.00
C8—C7—H7A	109.00	C48—C47—H47A	109.00
C6—C7—H7A	109.00	C48—C47—H47B	109.00
C6—C7—H7B	109.00	H47A—C47—H47B	108.00
H7A—C7—H7B	108.00	C47—C48—H48	109.00
C8—C7—H7B	109.00	C49—C48—H48	109.00
C9—C8—H8	109.00	C54—C48—H48	109.00
C14—C8—H8	109.00	C48—C49—H49	106.00
C7—C8—H8	109.00	C50—C49—H49	106.00

C11—C9—H9	107.00	C51—C49—H49	106.00
C8—C9—H9	107.00	C49—C51—H51A	109.00
C10—C9—H9	107.00	C49—C51—H51B	109.00
C12—C11—H11A	109.00	C52—C51—H51A	109.00
C12—C11—H11B	109.00	C52—C51—H51B	109.00
H11A—C11—H11B	108.00	H51A—C51—H51B	108.00
C9—C11—H11B	109.00	C51—C52—H52A	110.00
C9—C11—H11A	109.00	C51—C52—H52B	110.00
C11—C12—H12B	110.00	C53—C52—H52A	110.00
C11—C12—H12A	110.00	C53—C52—H52B	110.00
H12A—C12—H12B	108.00	H52A—C52—H52B	108.00
C13—C12—H12B	110.00	C48—C54—H54	106.00
C13—C12—H12A	110.00	C53—C54—H54	106.00
C13—C14—H14	106.00	C55—C54—H54	106.00
C15—C14—H14	106.00	C54—C55—H55A	111.00
C8—C14—H14	106.00	C54—C55—H55B	111.00
C16—C15—H15A	111.00	C56—C55—H55A	111.00
C14—C15—H15A	111.00	C56—C55—H55B	111.00
C14—C15—H15B	111.00	H55A—C55—H55B	109.00
H15A—C15—H15B	109.00	C55—C56—H56A	111.00
C16—C15—H15B	111.00	C55—C56—H56B	111.00
C15—C16—H16B	111.00	C57—C56—H56A	111.00
C15—C16—H16A	111.00	C57—C56—H56B	111.00
H16A—C16—H16B	109.00	H56A—C56—H56B	109.00
C17—C16—H16A	111.00	C53—C58—H58A	109.00
C17—C16—H16B	111.00	C53—C58—H58B	109.00
C13—C18—H18C	110.00	C53—C58—H58C	109.00
H18A—C18—H18B	109.00	H58A—C58—H58B	109.00
H18A—C18—H18C	109.00	H58A—C58—H58C	109.00
H18B—C18—H18C	109.00	H58B—C58—H58C	109.00
C13—C18—H18B	109.00	C50—C59—H59A	109.00
C13—C18—H18A	109.00	C50—C59—H59B	109.00
C10—C19—H19B	109.00	C50—C59—H59C	109.00
C10—C19—H19A	110.00	H59A—C59—H59B	110.00
H19A—C19—H19C	109.00	H59A—C59—H59C	109.00
H19B—C19—H19C	109.00	H59B—C59—H59C	109.00
C10—C19—H19C	109.00	C62—C61—H61A	109.00
H19A—C19—H19B	109.00	C62—C61—H61B	109.00
C30—C21—H21A	109.00	C70—C61—H61A	109.00
C22—C21—H21A	109.00	C70—C61—H61B	109.00
C22—C21—H21B	109.00	H61A—C61—H61B	108.00
H21A—C21—H21B	108.00	C61—C62—H62A	110.00
C30—C21—H21B	109.00	C61—C62—H62B	110.00
C23—C22—H22A	110.00	C63—C62—H62A	110.00
C23—C22—H22B	110.00	C63—C62—H62B	110.00
H22A—C22—H22B	108.00	H62A—C62—H62B	108.00
C21—C22—H22B	110.00	O15—C63—H63	110.00
C21—C22—H22A	110.00	C62—C63—H63	110.00
C24—C23—H23	110.00	C64—C63—H63	110.00

O5—C23—H23	110.00	C63—C64—H64A	109.00
C22—C23—H23	110.00	C63—C64—H64B	109.00
C25—C24—H24A	109.00	C65—C64—H64A	109.00
C25—C24—H24B	109.00	C65—C64—H64B	109.00
H24A—C24—H24B	108.00	H64A—C64—H64B	108.00
C23—C24—H24B	109.00	C65—C66—H66	118.00
C23—C24—H24A	109.00	C67—C66—H66	118.00
C27—C26—H26	117.00	C66—C67—H67A	109.00
C25—C26—H26	117.00	C66—C67—H67B	109.00
C28—C27—H27A	109.00	C68—C67—H67A	109.00
C28—C27—H27B	109.00	C68—C67—H67B	109.00
H27A—C27—H27B	108.00	H67A—C67—H67B	108.00
C26—C27—H27A	109.00	C67—C68—H68	109.00
C26—C27—H27B	109.00	C69—C68—H68	109.00
C34—C28—H28	109.00	C74—C68—H68	109.00
C27—C28—H28	109.00	C68—C69—H69	106.00
C29—C28—H28	109.00	C70—C69—H69	106.00
C31—C29—H29	106.00	C71—C69—H69	106.00
C28—C29—H29	106.00	C69—C71—H71A	109.00
C30—C29—H29	106.00	C69—C71—H71B	109.00
C29—C31—H31A	109.00	C72—C71—H71A	109.00
C32—C31—H31B	109.00	C72—C71—H71B	109.00
C29—C31—H31B	109.00	H71A—C71—H71B	108.00
C32—C31—H31A	109.00	C71—C72—H72A	110.00
H31A—C31—H31B	108.00	C71—C72—H72B	110.00
C33—C32—H32A	110.00	C73—C72—H72A	110.00
C33—C32—H32B	110.00	C73—C72—H72B	110.00
H32A—C32—H32B	108.00	H72A—C72—H72B	108.00
C31—C32—H32B	110.00	C68—C74—H74	106.00
C31—C32—H32A	110.00	C73—C74—H74	106.00
C35—C34—H34	105.00	C75—C74—H74	106.00
C28—C34—H34	105.00	C74—C75—H75A	112.00
C33—C34—H34	105.00	C74—C75—H75B	112.00
C36—C35—H35A	112.00	C76—C75—H75A	112.00
C36—C35—H35B	111.00	C76—C75—H75B	111.00
H35A—C35—H35B	109.00	H75A—C75—H75B	109.00
C34—C35—H35B	111.00	C75—C76—H76A	111.00
C34—C35—H35A	112.00	C75—C76—H76B	111.00
C35—C36—H36B	111.00	C77—C76—H76A	111.00
C35—C36—H36A	111.00	C77—C76—H76B	110.00
H36A—C36—H36B	109.00	H76A—C76—H76B	109.00
C37—C36—H36B	111.00	C73—C78—H78A	109.00
C37—C36—H36A	111.00	C73—C78—H78B	109.00
C33—C38—H38B	109.00	C73—C78—H78C	109.00
C33—C38—H38A	109.00	H78A—C78—H78B	109.00
H38A—C38—H38C	109.00	H78A—C78—H78C	109.00
C33—C38—H38C	109.00	H78B—C78—H78C	110.00
H38A—C38—H38B	109.00	C70—C79—H79A	109.00
H38B—C38—H38C	109.00	C70—C79—H79B	109.00

C30—C39—H39B	109.00	C70—C79—H79C	109.00
C30—C39—H39C	109.00	H79A—C79—H79B	109.00
H39A—C39—H39C	109.00	H79A—C79—H79C	110.00
H39B—C39—H39C	109.00	H79B—C79—H79C	109.00
C20—O1—C3—C2	84.0 (3)	C37—C33—C34—C28	179.0 (2)
C20—O1—C3—C4	−154.6 (2)	C37—C33—C34—C35	44.2 (2)
C3—O1—C20—O2	−5.2 (4)	C34—C33—C37—C36	−29.3 (3)
C3—O1—C20—C40	174.0 (2)	C28—C34—C35—C36	−173.7 (2)
C40—O5—C23—C22	79.6 (3)	C33—C34—C35—C36	−42.2 (2)
C40—O5—C23—C24	−159.6 (2)	C34—C35—C36—C37	22.6 (3)
C23—O5—C40—O4	−3.7 (4)	C35—C36—C37—O6	−174.2 (3)
C23—O5—C40—C20	176.8 (2)	C35—C36—C37—C33	4.3 (3)
C43—O11—C60—C80	171.9 (2)	C50—C41—C42—C43	−57.1 (3)
C60—O11—C43—C42	163.3 (2)	C42—C41—C50—C45	51.4 (3)
C60—O11—C43—C44	−76.5 (3)	C42—C41—C50—C49	170.6 (2)
C43—O11—C60—O12	−7.0 (4)	C42—C41—C50—C59	−66.9 (3)
C63—O15—C80—O14	8.5 (4)	C41—C42—C43—O11	175.0 (2)
C80—O15—C63—C64	−169.5 (2)	C41—C42—C43—C44	57.1 (3)
C63—O15—C80—C60	−172.3 (2)	O11—C43—C44—C45	−172.52 (19)
C80—O15—C63—C62	71.3 (3)	C42—C43—C44—C45	−55.1 (3)
C2—C1—C10—C19	−67.9 (3)	C43—C44—C45—C46	−127.7 (3)
C2—C1—C10—C9	170.4 (2)	C43—C44—C45—C50	52.2 (3)
C2—C1—C10—C5	50.2 (3)	C44—C45—C46—C47	−178.5 (2)
C10—C1—C2—C3	−57.4 (3)	C50—C45—C46—C47	1.6 (4)
C1—C2—C3—C4	59.5 (3)	C44—C45—C50—C41	−48.9 (3)
C1—C2—C3—O1	178.4 (2)	C44—C45—C50—C49	−167.8 (2)
O1—C3—C4—C5	−178.8 (2)	C44—C45—C50—C59	70.2 (3)
C2—C3—C4—C5	−57.4 (3)	C46—C45—C50—C41	131.0 (3)
C3—C4—C5—C10	53.5 (3)	C46—C45—C50—C49	12.2 (3)
C3—C4—C5—C6	−125.6 (3)	C46—C45—C50—C59	−109.9 (3)
C4—C5—C6—C7	−177.2 (2)	C45—C46—C47—C48	15.9 (4)
C10—C5—C6—C7	3.9 (4)	C46—C47—C48—C49	−46.0 (3)
C4—C5—C10—C1	−48.5 (3)	C46—C47—C48—C54	−166.6 (2)
C4—C5—C10—C9	−167.6 (2)	C47—C48—C49—C50	61.9 (3)
C4—C5—C10—C19	70.0 (3)	C47—C48—C49—C51	−169.67 (19)
C6—C5—C10—C1	130.5 (3)	C54—C48—C49—C50	−176.7 (2)
C6—C5—C10—C9	11.4 (4)	C54—C48—C49—C51	−48.3 (3)
C6—C5—C10—C19	−111.0 (3)	C47—C48—C54—C53	178.2 (2)
C5—C6—C7—C8	11.7 (4)	C47—C48—C54—C55	−57.2 (3)
C6—C7—C8—C14	−161.2 (2)	C49—C48—C54—C53	57.4 (3)
C6—C7—C8—C9	−41.5 (3)	C49—C48—C54—C55	−178.0 (2)
C7—C8—C9—C10	57.9 (3)	C48—C49—C50—C41	−161.6 (2)
C7—C8—C9—C11	−174.5 (2)	C48—C49—C50—C45	−43.4 (3)
C14—C8—C9—C11	−53.0 (3)	C48—C49—C50—C59	76.9 (3)
C7—C8—C14—C13	−178.1 (2)	C51—C49—C50—C41	69.9 (3)
C14—C8—C9—C10	179.4 (2)	C51—C49—C50—C45	−172.0 (2)
C9—C8—C14—C15	−174.2 (2)	C51—C49—C50—C59	−51.6 (3)
C7—C8—C14—C15	−52.5 (3)	C48—C49—C51—C52	47.5 (3)
C9—C8—C14—C13	60.2 (3)	C50—C49—C51—C52	175.8 (2)

C11—C9—C10—C19	−47.5 (3)	C49—C51—C52—C53	−51.4 (3)
C8—C9—C10—C1	−160.0 (2)	C51—C52—C53—C54	56.7 (3)
C8—C9—C10—C5	−41.7 (3)	C51—C52—C53—C57	168.5 (2)
C8—C9—C10—C19	79.4 (3)	C51—C52—C53—C58	−68.9 (3)
C11—C9—C10—C1	73.1 (3)	C52—C53—C54—C48	−62.7 (3)
C8—C9—C11—C12	53.0 (3)	C52—C53—C54—C55	164.8 (2)
C10—C9—C11—C12	−179.3 (2)	C57—C53—C54—C48	175.4 (2)
C11—C9—C10—C5	−168.6 (2)	C57—C53—C54—C55	43.0 (3)
C9—C11—C12—C13	−54.4 (3)	C58—C53—C54—C48	62.3 (3)
C11—C12—C13—C14	56.5 (3)	C58—C53—C54—C55	−70.2 (2)
C11—C12—C13—C18	−69.1 (3)	C52—C53—C57—O13	30.5 (4)
C11—C12—C13—C17	170.6 (2)	C52—C53—C57—C56	−147.6 (2)
C12—C13—C14—C8	−62.7 (3)	C54—C53—C57—O13	147.4 (3)
C14—C13—C17—C16	−22.9 (3)	C54—C53—C57—C56	−30.6 (3)
C18—C13—C17—O3	−82.3 (3)	C58—C53—C57—O13	−94.8 (3)
C18—C13—C17—C16	95.3 (3)	C58—C53—C57—C56	87.2 (3)
C18—C13—C14—C8	61.8 (3)	C48—C54—C55—C56	−168.0 (2)
C18—C13—C14—C15	−71.8 (3)	C53—C54—C55—C56	−39.3 (2)
C12—C13—C17—O3	41.8 (4)	C54—C55—C56—C57	19.2 (3)
C12—C13—C17—C16	−140.6 (2)	C55—C56—C57—O13	−170.7 (3)
C12—C13—C14—C15	163.7 (2)	C55—C56—C57—C53	7.4 (3)
C17—C13—C14—C8	173.0 (2)	O11—C60—C80—O14	−51.6 (4)
C17—C13—C14—C15	39.4 (3)	O11—C60—C80—O15	129.1 (2)
C14—C13—C17—O3	159.5 (3)	O12—C60—C80—O14	127.3 (3)
C8—C14—C15—C16	−170.7 (2)	O12—C60—C80—O15	−52.0 (4)
C13—C14—C15—C16	−40.9 (3)	C70—C61—C62—C63	−60.9 (3)
C14—C15—C16—C17	25.8 (3)	C62—C61—C70—C65	54.9 (3)
C15—C16—C17—O3	175.8 (3)	C62—C61—C70—C69	174.8 (2)
C15—C16—C17—C13	−1.8 (3)	C62—C61—C70—C79	−63.3 (3)
O1—C20—C40—O4	24.8 (4)	C61—C62—C63—O15	173.5 (2)
O1—C20—C40—O5	−155.7 (2)	C61—C62—C63—C64	57.5 (3)
O2—C20—C40—O5	23.5 (4)	O15—C63—C64—C65	−170.4 (2)
O2—C20—C40—O4	−156.0 (3)	C62—C63—C64—C65	−52.6 (3)
C22—C21—C30—C29	172.4 (2)	C63—C64—C65—C66	−131.3 (3)
C22—C21—C30—C39	−65.5 (3)	C63—C64—C65—C70	50.0 (3)
C30—C21—C22—C23	−60.4 (3)	C64—C65—C66—C67	−178.6 (2)
C22—C21—C30—C25	53.3 (3)	C70—C65—C66—C67	0.0 (4)
C21—C22—C23—C24	58.6 (3)	C64—C65—C70—C61	−49.2 (3)
C21—C22—C23—O5	175.2 (2)	C64—C65—C70—C69	−167.2 (2)
C22—C23—C24—C25	−53.5 (3)	C64—C65—C70—C79	70.5 (3)
O5—C23—C24—C25	−174.3 (2)	C66—C65—C70—C61	132.1 (3)
C23—C24—C25—C26	−131.4 (3)	C66—C65—C70—C69	14.1 (4)
C23—C24—C25—C30	49.0 (3)	C66—C65—C70—C79	−108.1 (3)
C24—C25—C26—C27	−177.9 (2)	C65—C66—C67—C68	14.4 (4)
C30—C25—C26—C27	1.6 (4)	C66—C67—C68—C69	−41.7 (3)
C24—C25—C30—C21	−47.5 (3)	C66—C67—C68—C74	−160.6 (2)
C24—C25—C30—C29	−166.0 (2)	C67—C68—C69—C70	57.0 (3)
C24—C25—C30—C39	71.5 (3)	C67—C68—C69—C71	−174.8 (2)
C26—C25—C30—C21	132.9 (3)	C74—C68—C69—C70	178.3 (2)

C26—C25—C30—C29	14.5 (4)	C74—C68—C69—C71	−53.6 (3)
C26—C25—C30—C39	−108.1 (3)	C67—C68—C74—C73	−179.6 (2)
C25—C26—C27—C28	13.1 (4)	C67—C68—C74—C75	−54.3 (3)
C26—C27—C28—C34	−162.8 (2)	C69—C68—C74—C73	59.5 (3)
C26—C27—C28—C29	−42.7 (3)	C69—C68—C74—C75	−175.3 (2)
C27—C28—C29—C31	−169.71 (19)	C68—C69—C70—C61	−160.0 (2)
C34—C28—C29—C30	−179.0 (2)	C68—C69—C70—C65	−42.3 (3)
C27—C28—C29—C30	60.6 (3)	C68—C69—C70—C79	78.4 (3)
C27—C28—C34—C33	175.2 (2)	C71—C69—C70—C61	71.9 (3)
C27—C28—C34—C35	−57.8 (3)	C71—C69—C70—C65	−170.4 (2)
C34—C28—C29—C31	−49.3 (3)	C71—C69—C70—C79	−49.7 (3)
C29—C28—C34—C33	54.8 (3)	C68—C69—C71—C72	52.8 (4)
C29—C28—C34—C35	−178.1 (2)	C70—C69—C71—C72	−178.8 (3)
C28—C29—C31—C32	52.3 (3)	C69—C71—C72—C73	−52.7 (4)
C28—C29—C30—C21	−162.9 (2)	C71—C72—C73—C74	55.1 (3)
C28—C29—C30—C25	−45.2 (3)	C71—C72—C73—C77	168.8 (3)
C28—C29—C30—C39	76.1 (3)	C71—C72—C73—C78	−72.1 (3)
C31—C29—C30—C21	68.0 (3)	C72—C73—C74—C68	−62.0 (3)
C31—C29—C30—C25	−174.3 (2)	C72—C73—C74—C75	164.4 (2)
C30—C29—C31—C32	−178.6 (2)	C77—C73—C74—C68	174.8 (2)
C31—C29—C30—C39	−53.0 (3)	C77—C73—C74—C75	41.3 (2)
C29—C31—C32—C33	−56.2 (3)	C78—C73—C74—C68	64.4 (3)
C31—C32—C33—C34	57.6 (3)	C78—C73—C74—C75	−69.1 (3)
C31—C32—C33—C37	168.4 (2)	C72—C73—C77—O16	36.4 (4)
C31—C32—C33—C38	−69.9 (3)	C72—C73—C77—C76	−143.6 (3)
C32—C33—C34—C28	−59.8 (3)	C74—C73—C77—O16	154.9 (3)
C32—C33—C34—C35	165.40 (19)	C74—C73—C77—C76	−25.1 (3)
C38—C33—C37—O6	−92.0 (3)	C78—C73—C77—O16	−87.3 (4)
C38—C33—C37—C36	89.6 (3)	C78—C73—C77—C76	92.8 (3)
C38—C33—C34—C28	66.6 (3)	C68—C74—C75—C76	−170.7 (3)
C38—C33—C34—C35	−68.2 (3)	C73—C74—C75—C76	−41.4 (3)
C32—C33—C37—O6	33.2 (4)	C74—C75—C76—C77	25.0 (3)
C32—C33—C37—C36	−145.3 (2)	C75—C76—C77—O16	−180.0 (3)
C34—C33—C37—O6	149.2 (3)	C75—C76—C77—C73	0.0 (3)

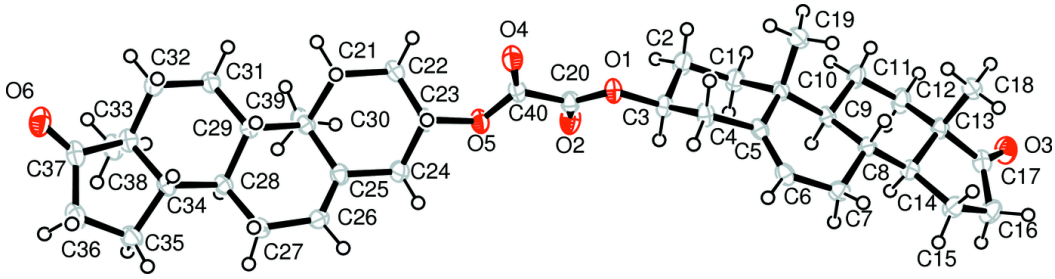
Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*, *y*+1/2, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) *x*+2, *y*, *z*; (v) −*x*+1, *y*−1/2, −*z*; (vi) *x*−2, *y*, *z*+1; (vii) −*x*−1, *y*−1/2, −*z*+1; (viii) *x*+2, *y*, *z*−1; (ix) *x*+1, *y*, *z*−1; (x) −*x*, *y*−1/2, −*z*+1; (xi) *x*−1, *y*, *z*+1; (xii) −*x*+1, *y*+1/2, −*z*; (xiii) −*x*−1, *y*+1/2, −*z*+1; (xiv) *x*−2, *y*, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4A···O3^{iii}	0.9900	2.5500	3.526 (3)	171.00
C21—H21A···O12^{x}	0.9900	2.3600	3.349 (3)	173.00
C34—H34···O2^{iii}	1.0000	2.3200	3.239 (3)	152.00
C47—H47A···O14^{i}	0.9900	2.5400	3.439 (3)	151.00
C62—H62B···O14	0.9900	2.5600	3.095 (3)	114.00
C64—H64A···O16^{i}	0.9900	2.5700	3.484 (4)	154.00

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

Fig. 1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C32
C31
C21
C22
O4
C20
O1
C2
C1
C19
C10
C11
C12
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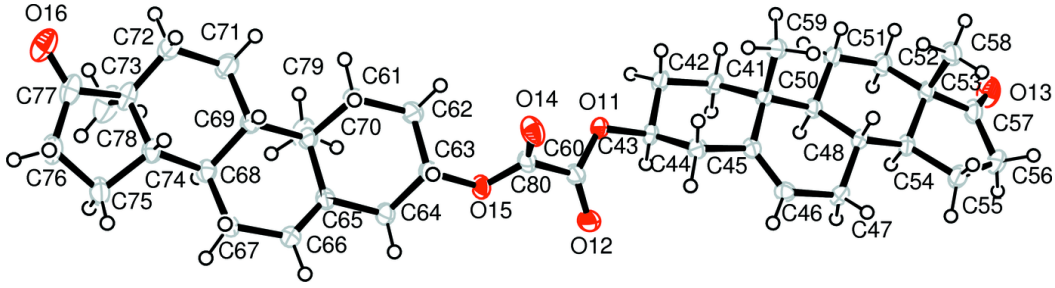
C33
C39
C23
C40
C3
C9
C13
C29
C30
O5
O2
C4
C5
O3
C37
C38
C28
C25
C24
C8
C17
C34
C26
C6
C14
C7
C16
C36
C35
C27
C15

Fig. 2


O16
C72
C71
C73
C79
C61
C77
C62
O14
O11
C69
C70
C78
C63
C60
C43
C42
C41
C59
C51
C58
C52
C50
C53
O13
C57
C76
C74
C68
C80
C44
C45
C48
C54
C56
C75
C65
C64
O15
C46
C55
C67
C66
O12
C47