organic compounds

5,11,17,23-Tetra-*tert*-butyl-25,26,27,28-tetramethoxycalix[4]arene tetrahydrofuran solvate

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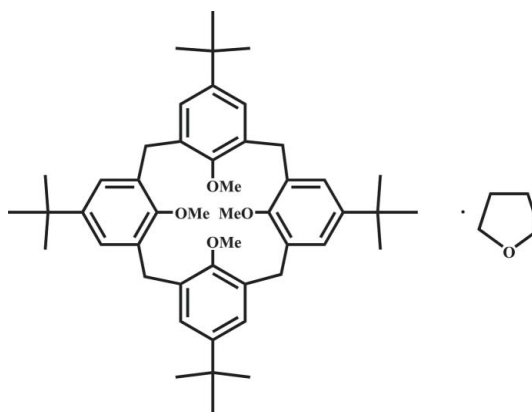Correspondence e-mail: edwin.weber@chemie.tu-freiberg.de

The asymmetric unit of the title compound, $C_{44}H_{64}O_4 \cdot C_4H_8O$, comprises two crystallographically independent calixarene molecules, which display a partial cone conformation, and two tetrahydrofuran molecules. The crystal packing is stabilized by C—H$\cdots\pi$ contacts involving the methoxy groups, while the solvent molecules are located in voids between the calixarene molecules. Two of the *tert*-butyl residues of each calixarene molecule are disordered over two positions [0.74/0.26 (ring B), 0.71/0.29 (ring C), 0.77/0.23 (ring C'), 0.67/0.33 (ring D')], resulting in bond distances that deviate from ideal values.

Related literature

The solvent-free title compound has been described as adopting the *paco*-conformation (Grootenhuis *et al.*, 1990). A corresponding sodium complex including toluene in the crystal structure shows a cone conformation (Bott *et al.*, 1986). A complex containing an aluminium alkyl species (Bott *et al.*, 1987) and a solvated complex with a nitrosyl compound (Rathore *et al.*, 2000) have also been reported. For the synthesis of the compound, see: Bitter *et al.* (1995). For other related literature, see: Gruber *et al.* (2007), Stumpf *et al.* (2003); Nishio (2004).

Experimental

Crystal data

$C_{48}H_{64}O_4 \cdot C_4H_8O$	$V = 9591.5$ (4) Å^3
$M_r = 777.10$	$Z = 8$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 16.9911$ (4) Å	$\mu = 0.07$ mm^{-1}
$b = 19.7724$ (5) Å	$T = 153$ (2) K
$c = 28.5530$ (7) Å	$0.55 \times 0.34 \times 0.10$ mm
$\beta = 90.8240$ (10)°	

Data collection

Bruker Kappa APEXII CCD diffractometer	97320 measured reflections
Absorption correction: multi-scan *SADABS* (Sheldrick, 2004)	19598 independent reflections
	8713 reflections with $I > 2\sigma(I)$
$T_{min} = 0.964$, $T_{max} = 0.993$	$R_{int} = 0.089$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.067$	35 restraints
$wR(F^2) = 0.215$	H-atom parameters constrained
$S = 1.00$	$\Delta\rho_{max} = 0.43$ e Å^{-3}
19598 reflections	$\Delta\rho_{min} = -0.43$ e Å^{-3}
1124 parameters	

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C14A—H14$D\cdots CgA^i$	0.99	2.93	3.817	149
C43—H43$A\cdots CgC'$	0.98	2.64	3.426	137
C48—H48$A\cdots CgA'^{ii}$	0.98	2.82	3.586	136
C48A—H48$D\cdots CgB'^{ii}$	0.98	2.84	3.580	133

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2051).

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supplementary materials

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Comment

The molecular geometry of the calixarene (Figure 1) is best described by a *partial*-cone conformation with opposite arene rings A and C differing only little from coplanarity (7.8 (1) and 8.1 (1)°, respectively), whereas the aromatic rings B and D include dihedral angles of 47.3 (1) and 55.7 (1)°, respectively. The solvent molecules are everything but located inside of the calixarene cavity offering not enough space for an accommodation. Hence the molecules of THF occupy interstitial lattice space between the calixarene molecules (Figure 2). Due to their hydrophobic surface, the packing of the calixarene molecules is primary stabilized by van-der-Waals interactions and weak C—H···π contacts (Nishio, 2004) involving methoxy groups and neighboring aromatic rings, with H···π (centroid of the aromatic ring) distances ranging from 2.64 to 2.93 Å. The *tert*-butyl residues are partially disordered over two positions, resulting in bond distances that deviate from ideal values.

Experimental

The title calixarene was sythesized from 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrahydroxycalix[4]arene following the literature procedure (Bitter *et al.*, 1995). Colourless prisms of the solvated calixarene suitable for X-ray diffraction were obtained by recrystallization from THF (m.p. 515–517 K).

Refinement

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 Å, and U_{iso}=1.2–1.5 U_{eq} (parent atom).

Figures

Fig. 1. Molecular presentation of (**I**) with THF as guest.
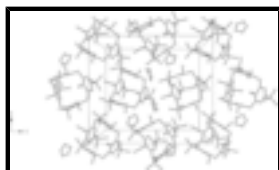
Fig. 2. Packing diagram, viewed down the *c* axis. H atoms have been omitted for clarity.

supplementary materials

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Crystal data

$C_{48}H_{64}O_4 \cdot C_4H_8O$	$Z = 8$
$M_r = 777.10$	$F_{000} = 3392$
Monoclinic, $P2_1/c$	$D_x = 1.076$ Mg m^{-3}
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 16.9911$ (4) Å	$\mu = 0.07$ mm^{-1}
$b = 19.7724$ (5) Å	$T = 153$ (2) K
$c = 28.5530$ (7) Å	Irregular, colourless
$\beta = 90.8240$ (10)°	$0.55 \times 0.34 \times 0.10$ mm
$V = 9591.5$ (4) Å^3	

Data collection

Bruker Kappa CCD APEXII area detector diffractometer	19598 independent reflections
Radiation source: fine-focus sealed tube	8713 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.089$
$T = 153(2)$ K	$\theta_{max} = 26.4°$
phi and ω scans	$\theta_{min} = 2.1°$
Absorption correction: multi-scan SADABS (Sheldrick, 2004)	$h = -21 \rightarrow 21$
$T_{min} = 0.964$, $T_{max} = 0.993$	$k = -24 \rightarrow 24$
97320 measured reflections	$l = -35 \rightarrow 35$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.067$	H-atom parameters constrained
$wR(F^2) = 0.215$	$w = 1/[\sigma^2(F_o^2) + (0.0872P)^2 + 5.146P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
19598 reflections	$\Delta\rho_{max} = 0.43$ e Å^{-3}
1124 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}
35 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
O1	−0.15340 (13)	0.99035 (11)	0.22112 (7)	0.0388 (5)	
O2	−0.05354 (12)	0.88434 (10)	0.27436 (7)	0.0361 (5)	
O3	0.10812 (12)	0.85837 (11)	0.23821 (7)	0.0383 (5)	
O4	0.08507 (13)	1.08372 (11)	0.26296 (7)	0.0436 (6)	
C1	−0.13829 (18)	1.02598 (16)	0.26245 (11)	0.0335 (7)	
C2	−0.09560 (18)	1.08577 (16)	0.26066 (11)	0.0341 (8)	
C3	−0.08175 (19)	1.12080 (17)	0.30216 (11)	0.0379 (8)	
H3	−0.0545	1.1627	0.3009	0.046*	
C4	−0.10612 (19)	1.09715 (17)	0.34560 (11)	0.0373 (8)	
C5	−0.14553 (18)	1.03535 (18)	0.34576 (11)	0.0392 (8)	
H5	−0.1623	1.0175	0.3749	0.047*	
C6	−0.16145 (18)	0.99860 (16)	0.30509 (11)	0.0355 (8)	
C7	−0.19955 (18)	0.92979 (17)	0.30864 (11)	0.0391 (8)	
H7A	−0.2103	0.9122	0.2767	0.047*	
H7B	−0.2506	0.9343	0.3247	0.047*	
C8	−0.07760 (19)	0.85774 (16)	0.31689 (11)	0.0336 (7)	
C9	−0.14826 (19)	0.87955 (16)	0.33526 (11)	0.0363 (8)	
C10	−0.1690 (2)	0.85571 (18)	0.37962 (11)	0.0427 (9)	
H10	−0.2171	0.8706	0.3928	0.051*	
C11	−0.1217 (2)	0.81098 (18)	0.40505 (11)	0.0439 (9)	
C12	−0.0518 (2)	0.79119 (17)	0.38510 (12)	0.0451 (9)	
H12	−0.0184	0.7609	0.4019	0.054*	
C13	−0.02819 (19)	0.81387 (16)	0.34125 (11)	0.0363 (8)	
C14	0.0521 (2)	0.79540 (16)	0.32200 (12)	0.0414 (8)	
H14A	0.0756	0.7586	0.3411	0.050*	
H14B	0.0458	0.7787	0.2895	0.050*	
C15	0.13096 (18)	0.88599 (16)	0.28130 (10)	0.0329 (7)	
C16	0.10686 (18)	0.85600 (16)	0.32258 (11)	0.0341 (8)	
C17	0.13075 (18)	0.88467 (17)	0.36480 (11)	0.0371 (8)	
H17	0.1145	0.8640	0.3931	0.045*	
C18	0.17744 (18)	0.94238 (17)	0.36743 (11)	0.0370 (8)	
C19	0.19748 (18)	0.97242 (17)	0.32510 (11)	0.0377 (8)	
H19	0.2278	1.0128	0.3258	0.045*	

C20	0.17507 (18)	0.94578 (17)	0.28180 (11)	0.0348 (8)
C21	0.19597 (19)	0.98214 (18)	0.23676 (11)	0.0402 (8)
H21A	0.2255	1.0238	0.2447	0.048*
H21B	0.2311	0.9528	0.2183	0.048*
C22	0.07082 (19)	1.04904 (16)	0.22110 (10)	0.0339 (8)
C23	0.12471 (19)	1.00099 (17)	0.20655 (11)	0.0357 (8)
C24	0.1097 (2)	0.96785 (18)	0.16449 (11)	0.0433 (9)
H24	0.1470	0.9359	0.1536	0.052*
C25	0.0418 (2)	0.97975 (18)	0.13755 (11)	0.0439 (9)
C26	−0.0119 (2)	1.02654 (17)	0.15477 (11)	0.0405 (8)
H26	−0.0592	1.0346	0.1375	0.049*
C27	0.00135 (19)	1.06191 (16)	0.19633 (11)	0.0358 (8)
C28	−0.0602 (2)	1.10990 (16)	0.21491 (11)	0.0395 (8)
H28A	−0.1028	1.1150	0.1912	0.047*
H28B	−0.0360	1.1549	0.2199	0.047*
C29	−0.0919 (2)	1.13723 (19)	0.39080 (12)	0.0495 (9)
C30	−0.0199 (3)	1.1823 (3)	0.38759 (16)	0.0960 (18)
H30A	−0.0124	1.2069	0.4171	0.144*
H30B	−0.0273	1.2147	0.3619	0.144*
H30C	0.0266	1.1545	0.3816	0.144*
C31	−0.1627 (3)	1.1840 (3)	0.39813 (16)	0.0858 (15)
H31A	−0.2102	1.1567	0.4024	0.129*
H31B	−0.1698	1.2132	0.3707	0.129*
H31C	−0.1534	1.2120	0.4260	0.129*
C32	−0.0821 (4)	1.0919 (3)	0.43280 (15)	0.1002 (19)
H32A	−0.1309	1.0666	0.4377	0.150*
H32B	−0.0701	1.1194	0.4606	0.150*
H32C	−0.0388	1.0601	0.4275	0.150*
C33	−0.2260 (2)	1.00904 (19)	0.19864 (13)	0.0519 (10)
H33A	−0.2699	0.9982	0.2192	0.078*
H33B	−0.2320	0.9841	0.1692	0.078*
H33C	−0.2258	1.0577	0.1922	0.078*
C34	−0.1457 (2)	0.7859 (2)	0.45364 (12)	0.0609 (11)
C35	−0.0813 (4)	0.8032 (6)	0.48852 (18)	0.117 (4)	0.736 (5)
H35A	−0.0982	0.7912	0.5201	0.175*	0.736 (5)
H35B	−0.0703	0.8518	0.4871	0.175*	0.736 (5)
H35C	−0.0336	0.7779	0.4809	0.175*	0.736 (5)
C36	−0.2226 (4)	0.8205 (4)	0.4704 (2)	0.087 (2)	0.736 (5)
H36A	−0.2656	0.8102	0.4483	0.130*	0.736 (5)
H36B	−0.2146	0.8696	0.4718	0.130*	0.736 (5)
H36C	−0.2358	0.8036	0.5016	0.130*	0.736 (5)
C37	−0.1631 (5)	0.7104 (3)	0.4495 (2)	0.102 (3)	0.736 (5)
H37A	−0.1800	0.6930	0.4799	0.153*	0.736 (5)
H37B	−0.1154	0.6865	0.4399	0.153*	0.736 (5)
H37C	−0.2050	0.7032	0.4261	0.153*	0.736 (5)
C35B	−0.1478 (13)	0.8463 (8)	0.4879 (5)	0.117 (4)	0.264 (5)
H35D	−0.1993	0.8684	0.4857	0.175*	0.264 (5)
H35E	−0.1065	0.8787	0.4798	0.175*	0.264 (5)
H35F	−0.1388	0.8300	0.5200	0.175*	0.264 (5)

C36B	−0.2243 (9)	0.7500 (12)	0.4532 (6)	0.087 (2)	0.264 (5)
H36D	−0.2403	0.7411	0.4855	0.130*	0.264 (5)
H36E	−0.2197	0.7071	0.4363	0.130*	0.264 (5)
H36F	−0.2639	0.7785	0.4377	0.130*	0.264 (5)
C37B	−0.0837 (10)	0.7368 (11)	0.4764 (7)	0.102 (3)	0.264 (5)
H37D	−0.0989	0.7264	0.5086	0.153*	0.264 (5)
H37E	−0.0318	0.7585	0.4767	0.153*	0.264 (5)
H37F	−0.0815	0.6949	0.4582	0.153*	0.264 (5)
C38	−0.0755 (2)	0.84537 (18)	0.23400 (11)	0.0462 (9)	
H38A	−0.0474	0.8021	0.2347	0.069*	
H38B	−0.0618	0.8703	0.2056	0.069*	
H38C	−0.1324	0.8371	0.2341	0.069*	
C39	0.2036 (2)	0.97132 (19)	0.41461 (12)	0.0501 (10)	
C40	0.2567 (5)	1.0319 (4)	0.4120 (2)	0.089 (3)	0.711 (5)
H40A	0.2721	1.0459	0.4438	0.134*	0.711 (5)
H40B	0.2288	1.0690	0.3963	0.134*	0.711 (5)
H40C	0.3038	1.0202	0.3944	0.134*	0.711 (5)
C41	0.1320 (4)	0.9878 (5)	0.4439 (2)	0.100 (3)	0.711 (5)
H41A	0.0968	0.9485	0.4445	0.149*	0.711 (5)
H41B	0.1040	1.0265	0.4300	0.149*	0.711 (5)
H41C	0.1490	0.9991	0.4759	0.149*	0.711 (5)
C42	0.2490 (5)	0.9159 (3)	0.4422 (2)	0.106 (3)	0.711 (5)
H42A	0.2591	0.9314	0.4743	0.159*	0.711 (5)
H42B	0.2991	0.9068	0.4268	0.159*	0.711 (5)
H42C	0.2174	0.8745	0.4428	0.159*	0.711 (5)
C40B	0.1795 (11)	1.0477 (5)	0.4116 (5)	0.089 (3)	0.289 (5)
H40D	0.1224	1.0512	0.4067	0.134*	0.289 (5)
H40E	0.2065	1.0691	0.3854	0.134*	0.289 (5)
H40F	0.1944	1.0705	0.4409	0.134*	0.289 (5)
C41B	0.1694 (13)	0.9378 (10)	0.4567 (5)	0.100 (3)	0.289 (5)
H41D	0.2005	0.9499	0.4847	0.149*	0.289 (5)
H41E	0.1704	0.8886	0.4525	0.149*	0.289 (5)
H41F	0.1150	0.9529	0.4606	0.149*	0.289 (5)
C42B	0.2938 (6)	0.9773 (11)	0.4150 (6)	0.106 (3)	0.289 (5)
H42D	0.3115	0.9998	0.4438	0.159*	0.289 (5)
H42E	0.3104	1.0038	0.3879	0.159*	0.289 (5)
H42F	0.3171	0.9320	0.4135	0.159*	0.289 (5)
C43	0.1636 (2)	0.81082 (19)	0.22012 (12)	0.0498 (9)	
H43A	0.2166	0.8305	0.2216	0.075*	
H43B	0.1497	0.8001	0.1875	0.075*	
H43C	0.1625	0.7694	0.2389	0.075*	
C44	0.0280 (2)	0.9422 (2)	0.09113 (12)	0.0610 (11)	
C45	0.0396 (6)	0.8663 (3)	0.0982 (2)	0.094 (3)	0.760 (5)
H45A	0.0325	0.8429	0.0682	0.141*	0.760 (5)
H45B	0.0010	0.8495	0.1206	0.141*	0.760 (5)
H45C	0.0929	0.8578	0.1105	0.141*	0.760 (5)
C46	0.0910 (5)	0.9669 (4)	0.05636 (19)	0.106 (3)	0.760 (5)
H46A	0.0865	0.9409	0.0272	0.159*	0.760 (5)
H46B	0.1436	0.9603	0.0702	0.159*	0.760 (5)

H46C	0.0828	1.0150	0.0497	0.159*	0.760 (5)
C47	−0.0536 (4)	0.9542 (4)	0.0700 (2)	0.106 (3)	0.760 (5)
H47A	−0.0582	1.0015	0.0600	0.159*	0.760 (5)
H47B	−0.0935	0.9444	0.0934	0.159*	0.760 (5)
H47C	−0.0614	0.9246	0.0428	0.159*	0.760 (5)
C45B	0.0905 (13)	0.8885 (11)	0.0799 (8)	0.094 (3)	0.240 (5)
H45D	0.0752	0.8644	0.0512	0.141*	0.240 (5)
H45E	0.0947	0.8563	0.1059	0.141*	0.240 (5)
H45F	0.1415	0.9106	0.0754	0.141*	0.240 (5)
C46B	0.024 (2)	0.9940 (9)	0.0512 (5)	0.106 (3)	0.240 (5)
H46D	0.0198	0.9703	0.0211	0.159*	0.240 (5)
H46E	0.0713	1.0220	0.0519	0.159*	0.240 (5)
H46F	−0.0226	1.0229	0.0552	0.159*	0.240 (5)
C47B	−0.0518 (9)	0.9049 (11)	0.0950 (7)	0.106 (3)	0.240 (5)
H47D	−0.0919	0.9365	0.1060	0.159*	0.240 (5)
H47E	−0.0465	0.8674	0.1172	0.159*	0.240 (5)
H47F	−0.0675	0.8872	0.0642	0.159*	0.240 (5)
C48	0.1269 (2)	1.1463 (2)	0.25673 (15)	0.0649 (12)	
H48A	0.1816	1.1366	0.2487	0.097*	
H48B	0.1257	1.1725	0.2858	0.097*	
H48C	0.1019	1.1723	0.2314	0.097*	
O1A	0.36984 (12)	0.13408 (10)	0.18620 (7)	0.0351 (5)	
O2A	0.52992 (12)	0.12776 (10)	0.23213 (7)	0.0331 (5)	
O3A	0.65424 (12)	0.22497 (11)	0.19345 (7)	0.0359 (5)	
O4A	0.44396 (13)	0.33962 (10)	0.23278 (7)	0.0355 (5)	
C1A	0.34875 (17)	0.16304 (15)	0.22862 (10)	0.0288 (7)	
C2A	0.32114 (17)	0.22910 (15)	0.22936 (10)	0.0278 (7)	
C3A	0.30071 (17)	0.25731 (15)	0.27185 (10)	0.0313 (7)	
H3A	0.2805	0.3021	0.2721	0.038*	
C4A	0.30834 (18)	0.22304 (16)	0.31417 (10)	0.0329 (7)	
C5A	0.33952 (18)	0.15806 (16)	0.31222 (10)	0.0325 (7)	
H5A	0.3470	0.1337	0.3406	0.039*	
C6A	0.36028 (17)	0.12711 (14)	0.27008 (10)	0.0277 (7)	
C7A	0.39993 (18)	0.05830 (15)	0.27118 (11)	0.0323 (7)	
H7A1	0.3662	0.0258	0.2880	0.039*	
H7A2	0.4062	0.0417	0.2387	0.039*	
C8A	0.54256 (18)	0.09510 (14)	0.27453 (10)	0.0272 (7)	
C9A	0.48007 (18)	0.06194 (14)	0.29534 (10)	0.0283 (7)	
C10A	0.49214 (18)	0.03426 (15)	0.33995 (10)	0.0309 (7)	
H10A	0.4498	0.0113	0.3544	0.037*	
C11A	0.56365 (18)	0.03896 (15)	0.36405 (10)	0.0308 (7)	
C12A	0.62497 (18)	0.07203 (15)	0.34132 (10)	0.0310 (7)	
H12A	0.6750	0.0747	0.3565	0.037*	
C13A	0.61550 (17)	0.10124 (14)	0.29717 (10)	0.0283 (7)	
C14A	0.68037 (18)	0.14352 (15)	0.27605 (11)	0.0337 (7)	
H14C	0.6881	0.1297	0.2431	0.040*	
H14D	0.7303	0.1354	0.2935	0.040*	
C15A	0.64640 (17)	0.25567 (16)	0.23713 (10)	0.0302 (7)	
C16A	0.66009 (17)	0.21852 (15)	0.27784 (10)	0.0301 (7)	

C17A	0.65084 (17)	0.25050 (16)	0.32083 (11)	0.0335 (8)
H17A	0.6600	0.2254	0.3487	0.040*
C18A	0.62860 (18)	0.31828 (17)	0.32436 (10)	0.0336 (7)
C19A	0.61382 (18)	0.35282 (16)	0.28317 (11)	0.0349 (8)
H19A	0.5981	0.3989	0.2848	0.042*
C20A	0.62105 (18)	0.32273 (16)	0.23925 (10)	0.0314 (7)
C21A	0.5979 (2)	0.36090 (17)	0.19510 (11)	0.0392 (8)
H21C	0.5820	0.4074	0.2037	0.047*
H21D	0.6444	0.3644	0.1747	0.047*
C22A	0.45741 (19)	0.31843 (15)	0.18711 (10)	0.0313 (7)
C23A	0.53117 (19)	0.32806 (16)	0.16762 (10)	0.0340 (8)
C24A	0.5438 (2)	0.30362 (17)	0.12281 (11)	0.0395 (8)
H24A	0.5938	0.3104	0.1092	0.047*
C25A	0.4863 (2)	0.26974 (17)	0.09707 (11)	0.0405 (8)
C26A	0.4137 (2)	0.25990 (16)	0.11828 (11)	0.0390 (8)
H26A	0.3737	0.2361	0.1016	0.047*
C27A	0.39789 (19)	0.28378 (15)	0.16311 (10)	0.0307 (7)
C28A	0.31798 (18)	0.27151 (16)	0.18485 (10)	0.0336 (7)
H28C	0.2836	0.2485	0.1616	0.040*
H28D	0.2937	0.3157	0.1921	0.040*
C29A	0.2854 (2)	0.25646 (18)	0.36083 (11)	0.0444 (9)
C30A	0.2990 (4)	0.3328 (2)	0.35876 (15)	0.115 (2)
H30D	0.2859	0.3531	0.3890	0.173*
H30E	0.2654	0.3525	0.3341	0.173*
H30F	0.3543	0.3418	0.3519	0.173*
C31A	0.1972 (2)	0.2438 (3)	0.36899 (14)	0.0800 (15)
H31D	0.1875	0.1951	0.3708	0.120*
H31E	0.1664	0.2631	0.3430	0.120*
H31F	0.1817	0.2653	0.3984	0.120*
C32A	0.3312 (3)	0.2265 (2)	0.40187 (12)	0.0687 (12)
H32D	0.3172	0.1787	0.4054	0.103*
H32E	0.3182	0.2511	0.4306	0.103*
H32F	0.3877	0.2304	0.3962	0.103*
C33A	0.3055 (2)	0.10413 (18)	0.16088 (11)	0.0492 (9)
H33D	0.2889	0.0627	0.1768	0.074*
H33E	0.3220	0.0931	0.1290	0.074*
H33F	0.2613	0.1360	0.1595	0.074*
C34A	0.5765 (2)	0.01112 (17)	0.41381 (10)	0.0373 (8)
C35A	0.5993 (3)	0.0694 (2)	0.44616 (12)	0.0655 (12)
H35G	0.6062	0.0524	0.4782	0.098*
H35H	0.5577	0.1037	0.4454	0.098*
H35I	0.6487	0.0895	0.4357	0.098*
C36A	0.5024 (2)	−0.0231 (2)	0.43275 (12)	0.0569 (11)
H36G	0.4855	−0.0591	0.4112	0.085*
H36H	0.4603	0.0104	0.4355	0.085*
H36I	0.5141	−0.0426	0.4636	0.085*
C37A	0.6422 (3)	−0.0417 (2)	0.41385 (13)	0.0659 (12)
H37G	0.6273	−0.0791	0.3930	0.099*
H37H	0.6505	−0.0590	0.4457	0.099*

H37I	0.6909	−0.0209	0.4028	0.099*	
C38A	0.5481 (2)	0.08957 (18)	0.19139 (11)	0.0436 (9)	
H38D	0.6034	0.0757	0.1928	0.065*	
H38E	0.5388	0.1174	0.1634	0.065*	
H38F	0.5144	0.0493	0.1899	0.065*	
C39A	0.6182 (2)	0.35151 (17)	0.37251 (11)	0.0414 (8)	
C40A	0.5866 (6)	0.4236 (3)	0.3692 (2)	0.101 (3)	0.768 (7)
H40G	0.5866	0.4440	0.4005	0.151*	0.768 (7)
H40H	0.5328	0.4228	0.3564	0.151*	0.768 (7)
H40I	0.6203	0.4503	0.3486	0.151*	0.768 (7)
C41A	0.5475 (5)	0.3188 (4)	0.3961 (2)	0.105 (3)	0.768 (7)
H41G	0.5516	0.2695	0.3937	0.157*	0.768 (7)
H41H	0.4989	0.3340	0.3806	0.157*	0.768 (7)
H41I	0.5469	0.3319	0.4292	0.157*	0.768 (7)
C42A	0.6893 (5)	0.3382 (6)	0.4041 (3)	0.128 (5)	0.768 (7)
H42G	0.7351	0.3623	0.3919	0.192*	0.768 (7)
H42H	0.7003	0.2895	0.4048	0.192*	0.768 (7)
H42I	0.6784	0.3541	0.4358	0.192*	0.768 (7)
C40C	0.648 (2)	0.4246 (7)	0.3702 (9)	0.101 (3)	0.232 (7)
H40J	0.6491	0.4441	0.4018	0.151*	0.232 (7)
H40K	0.6129	0.4513	0.3500	0.151*	0.232 (7)
H40L	0.7013	0.4251	0.3575	0.151*	0.232 (7)
C41C	0.6108 (17)	0.2987 (10)	0.4111 (6)	0.105 (3)	0.232 (7)
H41J	0.6499	0.2629	0.4064	0.157*	0.232 (7)
H41K	0.5579	0.2790	0.4100	0.157*	0.232 (7)
H41L	0.6200	0.3201	0.4416	0.157*	0.232 (7)
C42C	0.6973 (11)	0.3843 (19)	0.3849 (11)	0.128 (5)	0.232 (7)
H42J	0.6950	0.4042	0.4162	0.192*	0.232 (7)
H42K	0.7089	0.4198	0.3620	0.192*	0.232 (7)
H42L	0.7389	0.3500	0.3843	0.192*	0.232 (7)
C43A	0.7308 (2)	0.2326 (2)	0.17395 (12)	0.0561 (10)	
H43D	0.7448	0.2807	0.1731	0.084*	
H43E	0.7308	0.2143	0.1421	0.084*	
H43F	0.7694	0.2081	0.1933	0.084*	
C44A	0.5023 (2)	0.24116 (18)	0.04822 (11)	0.0513 (10)	
C45A	0.4457 (4)	0.2705 (5)	0.01292 (18)	0.085 (2)	0.667 (4)
H45G	0.4428	0.3197	0.0172	0.127*	0.667 (4)
H45H	0.3934	0.2507	0.0173	0.127*	0.667 (4)
H45I	0.4638	0.2604	−0.0187	0.127*	0.667 (4)
C46A	0.5840 (4)	0.2696 (4)	0.0295 (2)	0.083 (2)	0.667 (4)
H46G	0.5925	0.2530	−0.0024	0.124*	0.667 (4)
H46H	0.6270	0.2540	0.0501	0.124*	0.667 (4)
H46I	0.5827	0.3191	0.0294	0.124*	0.667 (4)
C47A	0.5139 (7)	0.1660 (3)	0.0510 (3)	0.102 (4)	0.667 (4)
H47G	0.5353	0.1496	0.0214	0.153*	0.667 (4)
H47H	0.4633	0.1440	0.0567	0.153*	0.667 (4)
H47I	0.5507	0.1554	0.0767	0.153*	0.667 (4)
C45C	0.4285 (7)	0.1990 (8)	0.0282 (4)	0.085 (2)	0.333 (4)
H45J	0.3823	0.2285	0.0261	0.127*	0.333 (4)

H45K	0.4175	0.1611	0.0492	0.127*	0.333 (4)
H45L	0.4406	0.1816	−0.0030	0.127*	0.333 (4)
C46C	0.5114 (11)	0.2966 (6)	0.0132 (4)	0.083 (2)	0.333 (4)
H46J	0.5506	0.3292	0.0247	0.124*	0.333 (4)
H46K	0.4608	0.3195	0.0085	0.124*	0.333 (4)
H46L	0.5287	0.2775	−0.0166	0.124*	0.333 (4)
C47C	0.5683 (9)	0.1901 (8)	0.0516 (6)	0.102 (4)	0.333 (4)
H47J	0.5781	0.1711	0.0206	0.153*	0.333 (4)
H47K	0.5534	0.1537	0.0731	0.153*	0.333 (4)
H47L	0.6161	0.2123	0.0635	0.153*	0.333 (4)
C48A	0.4173 (2)	0.40758 (17)	0.23744 (12)	0.0456 (9)	
H48D	0.4566	0.4385	0.2246	0.068*	
H48E	0.4095	0.4179	0.2706	0.068*	
H48F	0.3674	0.4132	0.2202	0.068*	
O1H	0.1091 (7)	0.6645 (6)	0.4325 (3)	0.295 (5)	
C1H	0.1302 (8)	0.7257 (5)	0.4554 (5)	0.224 (6)	
H1H1	0.1373	0.7629	0.4326	0.268*	
H1H2	0.0899	0.7392	0.4783	0.268*	
C2H	0.2000 (7)	0.7098 (7)	0.4774 (4)	0.218 (5)	
H2H1	0.2391	0.7458	0.4714	0.262*	
H2H2	0.1919	0.7074	0.5117	0.262*	
C3H	0.2283 (5)	0.6494 (5)	0.4619 (3)	0.154 (3)	
H3H1	0.2362	0.6177	0.4883	0.185*	
H3H2	0.2791	0.6558	0.4459	0.185*	
C4H	0.1719 (5)	0.6251 (4)	0.4310 (3)	0.141 (3)	
H4H1	0.1931	0.6245	0.3989	0.169*	
H4H2	0.1575	0.5783	0.4397	0.169*	
O1G	0.2796 (4)	0.4781 (3)	0.4310 (2)	0.196 (2)	
C1G	0.3615 (6)	0.4966 (5)	0.4241 (4)	0.229 (6)	
H1G1	0.3660	0.5439	0.4131	0.275*	
H1G2	0.3866	0.4663	0.4011	0.275*	
C2G	0.3978 (8)	0.4881 (8)	0.4717 (5)	0.296 (10)	
H2G1	0.4318	0.5278	0.4782	0.355*	
H2G2	0.4321	0.4476	0.4713	0.355*	
C3G	0.3404 (9)	0.4807 (9)	0.5113 (4)	0.393 (16)	
H3G1	0.3230	0.5245	0.5245	0.472*	
H3G2	0.3591	0.4500	0.5365	0.472*	
C4G	0.2803 (7)	0.4485 (6)	0.4782 (3)	0.239 (6)	
H4G1	0.2917	0.3996	0.4758	0.286*	
H4G2	0.2273	0.4535	0.4917	0.286*	

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0353 (13)	0.0404 (13)	0.0406 (13)	0.0047 (11)	−0.0054 (10)	−0.0056 (10)
O2	0.0374 (13)	0.0366 (13)	0.0343 (12)	−0.0043 (11)	0.0022 (10)	0.0016 (10)
O3	0.0329 (12)	0.0433 (13)	0.0387 (13)	0.0079 (11)	−0.0038 (10)	−0.0046 (10)
O4	0.0389 (13)	0.0469 (14)	0.0449 (13)	−0.0095 (12)	0.0001 (11)	−0.0089 (11)

C1	0.0276 (17)	0.0337 (19)	0.0392 (19)	0.0059 (15)	−0.0019 (15)	−0.0033 (15)
C2	0.0306 (18)	0.0296 (18)	0.0420 (19)	0.0071 (15)	−0.0025 (15)	0.0013 (15)
C3	0.0327 (18)	0.0340 (19)	0.047 (2)	0.0019 (16)	−0.0030 (16)	0.0001 (16)
C4	0.0299 (18)	0.042 (2)	0.0398 (19)	0.0011 (16)	−0.0018 (15)	−0.0031 (16)
C5	0.0271 (17)	0.050 (2)	0.0402 (19)	−0.0008 (17)	0.0055 (15)	−0.0011 (17)
C6	0.0228 (17)	0.041 (2)	0.043 (2)	0.0012 (15)	0.0020 (15)	−0.0035 (16)
C7	0.0248 (17)	0.047 (2)	0.0455 (19)	−0.0043 (16)	0.0020 (15)	−0.0034 (16)
C8	0.0346 (18)	0.0312 (18)	0.0349 (18)	−0.0098 (16)	−0.0013 (15)	−0.0003 (14)
C9	0.0312 (18)	0.0363 (19)	0.0412 (19)	−0.0121 (16)	−0.0011 (15)	−0.0033 (15)
C10	0.0353 (19)	0.052 (2)	0.041 (2)	−0.0152 (18)	0.0027 (16)	−0.0032 (17)
C11	0.044 (2)	0.051 (2)	0.0365 (19)	−0.0204 (19)	−0.0058 (17)	0.0075 (17)
C12	0.048 (2)	0.043 (2)	0.044 (2)	−0.0107 (18)	−0.0070 (18)	0.0097 (17)
C13	0.0354 (19)	0.0300 (18)	0.043 (2)	−0.0103 (16)	−0.0036 (16)	−0.0004 (15)
C14	0.043 (2)	0.0346 (19)	0.046 (2)	0.0027 (17)	−0.0044 (17)	0.0039 (16)
C15	0.0249 (16)	0.0407 (19)	0.0329 (18)	0.0090 (16)	−0.0038 (14)	−0.0024 (15)
C16	0.0280 (17)	0.0318 (18)	0.0424 (19)	0.0042 (15)	−0.0024 (15)	0.0007 (15)
C17	0.0328 (18)	0.042 (2)	0.0365 (19)	0.0035 (17)	0.0038 (15)	0.0048 (16)
C18	0.0300 (18)	0.046 (2)	0.0354 (18)	−0.0005 (17)	0.0001 (15)	−0.0024 (16)
C19	0.0279 (17)	0.044 (2)	0.042 (2)	−0.0036 (16)	−0.0030 (15)	−0.0012 (16)
C20	0.0225 (16)	0.046 (2)	0.0364 (18)	0.0032 (16)	−0.0001 (14)	−0.0010 (15)
C21	0.0306 (18)	0.050 (2)	0.0403 (19)	−0.0018 (17)	0.0049 (15)	0.0018 (16)
C22	0.0371 (19)	0.0337 (18)	0.0308 (17)	−0.0060 (16)	0.0019 (15)	0.0008 (14)
C23	0.0291 (17)	0.042 (2)	0.0356 (18)	−0.0024 (16)	0.0027 (15)	0.0039 (15)
C24	0.044 (2)	0.050 (2)	0.0359 (19)	0.0085 (18)	0.0038 (17)	0.0021 (17)
C25	0.051 (2)	0.046 (2)	0.0342 (19)	0.0061 (19)	−0.0018 (17)	−0.0008 (16)
C26	0.042 (2)	0.044 (2)	0.0350 (18)	0.0033 (18)	−0.0054 (16)	0.0064 (16)
C27	0.0376 (19)	0.0342 (18)	0.0357 (18)	−0.0020 (16)	0.0028 (16)	0.0055 (15)
C28	0.043 (2)	0.0338 (19)	0.0417 (19)	0.0000 (17)	−0.0001 (16)	0.0053 (15)
C29	0.050 (2)	0.055 (2)	0.044 (2)	−0.008 (2)	−0.0041 (18)	−0.0073 (18)
C30	0.091 (4)	0.128 (4)	0.069 (3)	−0.053 (4)	0.000 (3)	−0.035 (3)
C31	0.087 (4)	0.098 (4)	0.073 (3)	0.015 (3)	0.000 (3)	−0.041 (3)
C32	0.158 (5)	0.090 (4)	0.052 (3)	−0.021 (4)	−0.035 (3)	0.001 (3)
C33	0.044 (2)	0.055 (2)	0.056 (2)	0.0060 (19)	−0.0189 (19)	−0.0042 (19)
C34	0.051 (2)	0.091 (3)	0.040 (2)	−0.019 (2)	−0.0038 (19)	0.015 (2)
C35	0.073 (5)	0.248 (11)	0.029 (3)	−0.044 (6)	−0.012 (3)	0.022 (5)
C36	0.069 (4)	0.140 (6)	0.052 (4)	−0.012 (5)	0.017 (3)	0.023 (4)
C37	0.122 (7)	0.106 (6)	0.078 (5)	−0.043 (5)	0.014 (4)	0.045 (4)
C35B	0.073 (5)	0.248 (11)	0.029 (3)	−0.044 (6)	−0.012 (3)	0.022 (5)
C36B	0.069 (4)	0.140 (6)	0.052 (4)	−0.012 (5)	0.017 (3)	0.023 (4)
C37B	0.122 (7)	0.106 (6)	0.078 (5)	−0.043 (5)	0.014 (4)	0.045 (4)
C38	0.045 (2)	0.053 (2)	0.041 (2)	0.0009 (19)	−0.0040 (17)	−0.0036 (17)
C39	0.045 (2)	0.064 (3)	0.042 (2)	−0.011 (2)	−0.0029 (18)	−0.0028 (19)
C40	0.109 (6)	0.112 (5)	0.047 (3)	−0.066 (6)	−0.004 (4)	−0.011 (3)
C41	0.099 (6)	0.140 (8)	0.060 (4)	−0.024 (5)	0.022 (4)	−0.048 (5)
C42	0.141 (7)	0.088 (5)	0.086 (5)	0.017 (5)	−0.069 (5)	−0.009 (4)
C40B	0.109 (6)	0.112 (5)	0.047 (3)	−0.066 (6)	−0.004 (4)	−0.011 (3)
C41B	0.099 (6)	0.140 (8)	0.060 (4)	−0.024 (5)	0.022 (4)	−0.048 (5)
C42B	0.141 (7)	0.088 (5)	0.086 (5)	0.017 (5)	−0.069 (5)	−0.009 (4)
C43	0.046 (2)	0.056 (2)	0.047 (2)	0.014 (2)	0.0007 (18)	−0.0121 (18)

C44	0.075 (3)	0.069 (3)	0.038 (2)	0.023 (2)	−0.014 (2)	−0.0096 (19)
C45	0.149 (8)	0.061 (4)	0.070 (5)	0.022 (5)	−0.041 (5)	−0.024 (3)
C46	0.148 (8)	0.135 (7)	0.036 (3)	0.014 (6)	0.020 (4)	−0.011 (4)
C47	0.118 (5)	0.124 (7)	0.074 (5)	0.057 (5)	−0.064 (4)	−0.053 (4)
C45B	0.149 (8)	0.061 (4)	0.070 (5)	0.022 (5)	−0.041 (5)	−0.024 (3)
C46B	0.148 (8)	0.135 (7)	0.036 (3)	0.014 (6)	0.020 (4)	−0.011 (4)
C47B	0.118 (5)	0.124 (7)	0.074 (5)	0.057 (5)	−0.064 (4)	−0.053 (4)
C48	0.051 (2)	0.053 (3)	0.091 (3)	−0.018 (2)	0.006 (2)	−0.014 (2)
O1A	0.0370 (12)	0.0353 (12)	0.0330 (12)	0.0027 (11)	−0.0001 (10)	−0.0036 (10)
O2A	0.0340 (12)	0.0344 (12)	0.0310 (12)	0.0006 (10)	0.0010 (10)	0.0031 (10)
O3A	0.0331 (12)	0.0413 (13)	0.0334 (12)	−0.0039 (11)	0.0045 (10)	−0.0019 (10)
O4A	0.0470 (14)	0.0302 (12)	0.0293 (12)	−0.0009 (11)	0.0018 (10)	−0.0018 (9)
C1A	0.0228 (16)	0.0329 (18)	0.0308 (17)	−0.0014 (14)	0.0029 (13)	−0.0040 (14)
C2A	0.0215 (15)	0.0289 (17)	0.0330 (17)	0.0019 (14)	−0.0021 (13)	0.0018 (14)
C3A	0.0276 (17)	0.0251 (16)	0.0413 (19)	−0.0007 (14)	0.0011 (14)	−0.0026 (14)
C4A	0.0308 (17)	0.0343 (19)	0.0334 (17)	−0.0076 (16)	0.0003 (14)	−0.0033 (15)
C5A	0.0305 (17)	0.0345 (19)	0.0328 (17)	−0.0047 (15)	0.0020 (14)	0.0053 (14)
C6A	0.0216 (15)	0.0260 (17)	0.0356 (18)	−0.0023 (14)	−0.0005 (13)	0.0009 (14)
C7A	0.0315 (17)	0.0277 (17)	0.0377 (18)	−0.0033 (15)	0.0003 (15)	0.0058 (14)
C8A	0.0296 (17)	0.0220 (16)	0.0299 (16)	0.0024 (14)	−0.0005 (14)	0.0021 (13)
C9A	0.0301 (17)	0.0205 (15)	0.0343 (17)	−0.0002 (14)	−0.0007 (14)	−0.0005 (13)
C10A	0.0319 (17)	0.0265 (17)	0.0346 (18)	−0.0006 (15)	0.0058 (15)	−0.0006 (14)
C11A	0.0364 (18)	0.0241 (16)	0.0321 (17)	−0.0008 (15)	0.0039 (15)	−0.0008 (13)
C12A	0.0291 (17)	0.0294 (17)	0.0343 (17)	0.0018 (15)	−0.0043 (14)	−0.0005 (14)
C13A	0.0277 (17)	0.0228 (16)	0.0344 (17)	0.0000 (14)	0.0021 (14)	−0.0025 (13)
C14A	0.0254 (16)	0.0389 (19)	0.0368 (18)	0.0020 (15)	0.0025 (14)	0.0002 (15)
C15A	0.0255 (16)	0.0361 (19)	0.0290 (17)	−0.0076 (15)	0.0030 (13)	0.0003 (14)
C16A	0.0218 (15)	0.0327 (18)	0.0358 (18)	−0.0049 (14)	0.0039 (14)	0.0034 (14)
C17A	0.0283 (17)	0.0379 (19)	0.0343 (18)	−0.0079 (16)	0.0011 (14)	0.0078 (15)
C18A	0.0287 (17)	0.0388 (19)	0.0333 (18)	−0.0051 (16)	0.0026 (14)	−0.0014 (15)
C19A	0.0348 (18)	0.0275 (17)	0.0424 (19)	−0.0047 (15)	0.0039 (15)	0.0000 (15)
C20A	0.0287 (17)	0.0309 (18)	0.0347 (18)	−0.0076 (15)	−0.0007 (14)	0.0035 (14)
C21A	0.041 (2)	0.0365 (19)	0.0400 (19)	−0.0049 (17)	0.0048 (16)	0.0054 (15)
C22A	0.0416 (19)	0.0281 (17)	0.0242 (16)	0.0054 (16)	−0.0006 (15)	0.0036 (13)
C23A	0.0394 (19)	0.0326 (18)	0.0299 (17)	0.0018 (16)	0.0021 (15)	0.0095 (14)
C24A	0.045 (2)	0.043 (2)	0.0301 (18)	0.0074 (18)	0.0066 (16)	0.0094 (15)
C25A	0.053 (2)	0.040 (2)	0.0285 (17)	0.0138 (18)	−0.0003 (17)	0.0056 (15)
C26A	0.053 (2)	0.0300 (18)	0.0342 (18)	0.0054 (17)	−0.0090 (17)	0.0006 (14)
C27A	0.0381 (18)	0.0263 (17)	0.0277 (16)	0.0052 (15)	−0.0027 (15)	0.0050 (13)
C28A	0.0325 (18)	0.0328 (18)	0.0354 (17)	0.0022 (15)	−0.0055 (14)	−0.0006 (14)
C29A	0.054 (2)	0.044 (2)	0.0354 (19)	−0.0036 (19)	0.0070 (17)	−0.0037 (16)
C30A	0.237 (7)	0.050 (3)	0.059 (3)	−0.031 (4)	0.029 (4)	−0.022 (2)
C31A	0.057 (3)	0.130 (4)	0.053 (3)	0.020 (3)	0.014 (2)	−0.020 (3)
C32A	0.070 (3)	0.094 (3)	0.042 (2)	0.002 (3)	−0.006 (2)	−0.018 (2)
C33A	0.061 (2)	0.047 (2)	0.039 (2)	−0.010 (2)	−0.0044 (19)	−0.0083 (17)
C34A	0.041 (2)	0.040 (2)	0.0304 (17)	0.0023 (17)	−0.0002 (15)	−0.0002 (15)
C35A	0.086 (3)	0.073 (3)	0.037 (2)	−0.018 (3)	−0.002 (2)	−0.004 (2)
C36A	0.064 (3)	0.065 (3)	0.042 (2)	−0.013 (2)	−0.0001 (19)	0.0107 (19)
C37A	0.073 (3)	0.076 (3)	0.049 (2)	0.023 (2)	0.004 (2)	0.021 (2)

C38A	0.046 (2)	0.050 (2)	0.0352 (19)	−0.0011 (18)	0.0018 (16)	−0.0004 (16)
C39A	0.047 (2)	0.043 (2)	0.0340 (18)	−0.0049 (18)	0.0062 (17)	−0.0011 (15)
C40A	0.180 (10)	0.072 (4)	0.050 (3)	0.047 (5)	0.020 (6)	−0.015 (3)
C41A	0.099 (6)	0.143 (6)	0.075 (4)	−0.040 (6)	0.064 (5)	−0.039 (4)
C42A	0.100 (5)	0.207 (12)	0.076 (6)	0.061 (7)	−0.044 (5)	−0.087 (7)
C40C	0.180 (10)	0.072 (4)	0.050 (3)	0.047 (5)	0.020 (6)	−0.015 (3)
C41C	0.099 (6)	0.143 (6)	0.075 (4)	−0.040 (6)	0.064 (5)	−0.039 (4)
C42C	0.100 (5)	0.207 (12)	0.076 (6)	0.061 (7)	−0.044 (5)	−0.087 (7)
C43A	0.047 (2)	0.077 (3)	0.045 (2)	−0.010 (2)	0.0170 (18)	−0.008 (2)
C44A	0.065 (3)	0.057 (2)	0.0324 (19)	0.013 (2)	0.0026 (18)	−0.0063 (17)
C45A	0.086 (5)	0.139 (6)	0.029 (3)	0.027 (5)	−0.002 (3)	−0.018 (4)
C46A	0.084 (5)	0.123 (6)	0.042 (3)	−0.013 (5)	0.023 (3)	−0.020 (3)
C47A	0.193 (12)	0.053 (5)	0.060 (3)	0.003 (5)	0.036 (7)	−0.022 (4)
C45C	0.086 (5)	0.139 (6)	0.029 (3)	0.027 (5)	−0.002 (3)	−0.018 (4)
C46C	0.084 (5)	0.123 (6)	0.042 (3)	−0.013 (5)	0.023 (3)	−0.020 (3)
C47C	0.193 (12)	0.053 (5)	0.060 (3)	0.003 (5)	0.036 (7)	−0.022 (4)
C48A	0.054 (2)	0.038 (2)	0.045 (2)	−0.0008 (18)	0.0059 (18)	−0.0078 (16)
O1H	0.358 (14)	0.225 (10)	0.297 (10)	0.116 (10)	−0.117 (9)	−0.033 (8)
C1H	0.247 (14)	0.092 (6)	0.331 (15)	0.086 (8)	−0.040 (11)	−0.020 (8)
C2H	0.184 (11)	0.211 (12)	0.260 (13)	0.019 (9)	0.020 (9)	−0.128 (10)
C3H	0.120 (6)	0.150 (7)	0.190 (8)	−0.005 (6)	−0.033 (6)	−0.033 (6)
C4H	0.119 (6)	0.128 (7)	0.175 (7)	−0.041 (6)	0.000 (6)	0.010 (6)
O1G	0.205 (7)	0.186 (6)	0.198 (6)	0.015 (5)	0.005 (5)	−0.026 (5)
C1G	0.160 (9)	0.199 (11)	0.332 (17)	−0.079 (9)	0.101 (11)	−0.102 (11)
C2G	0.310 (19)	0.248 (15)	0.325 (19)	−0.050 (13)	−0.202 (18)	0.076 (15)
C3G	0.67 (4)	0.36 (2)	0.141 (10)	0.24 (2)	−0.105 (16)	−0.117 (14)
C4G	0.375 (18)	0.246 (12)	0.096 (6)	0.009 (12)	0.081 (9)	0.031 (7)

Geometric parameters (Å, °)

O1—C1	1.395 (4)	O4A—C48A	1.425 (4)
O1—C33	1.431 (4)	C1A—C2A	1.388 (4)
O2—C8	1.390 (3)	C1A—C6A	1.392 (4)
O2—C38	1.431 (4)	C2A—C3A	1.384 (4)
O3—C15	1.396 (4)	C2A—C28A	1.523 (4)
O3—C43	1.433 (4)	C3A—C4A	1.390 (4)
O4—C22	1.396 (4)	C3A—H3A	0.9500
O4—C48	1.439 (4)	C4A—C5A	1.391 (4)
C1—C2	1.388 (4)	C4A—C29A	1.542 (4)
C1—C6	1.394 (4)	C5A—C6A	1.400 (4)
C2—C3	1.390 (4)	C5A—H5A	0.9500
C2—C28	1.523 (4)	C6A—C7A	1.518 (4)
C3—C4	1.394 (4)	C7A—C9A	1.519 (4)
C3—H3	0.9500	C7A—H7A1	0.9900
C4—C5	1.394 (5)	C7A—H7A2	0.9900
C4—C29	1.531 (5)	C8A—C9A	1.389 (4)
C5—C6	1.393 (4)	C8A—C13A	1.395 (4)
C5—H5	0.9500	C9A—C10A	1.399 (4)
C6—C7	1.511 (4)	C10A—C11A	1.391 (4)

C7—C9	1.518 (5)	C10A—H10A	0.9500
C7—H7A	0.9900	C11A—C12A	1.398 (4)
C7—H7B	0.9900	C11A—C34A	1.536 (4)
C8—C13	1.387 (4)	C12A—C13A	1.394 (4)
C8—C9	1.386 (4)	C12A—H12A	0.9500
C9—C10	1.401 (4)	C13A—C14A	1.515 (4)
C10—C11	1.392 (5)	C14A—C16A	1.523 (4)
C10—H10	0.9500	C14A—H14C	0.9900
C11—C12	1.382 (5)	C14A—H14D	0.9900
C11—C34	1.534 (5)	C15A—C16A	1.392 (4)
C12—C13	1.394 (4)	C15A—C20A	1.396 (4)
C12—H12	0.9500	C16A—C17A	1.392 (4)
C13—C14	1.523 (5)	C17A—C18A	1.396 (4)
C14—C16	1.517 (4)	C17A—H17A	0.9500
C14—H14A	0.9900	C18A—C19A	1.380 (4)
C14—H14B	0.9900	C18A—C39A	1.536 (4)
C15—C16	1.387 (4)	C19A—C20A	1.395 (4)
C15—C20	1.400 (4)	C19A—H19A	0.9500
C16—C17	1.387 (4)	C20A—C21A	1.517 (4)
C17—C18	1.391 (4)	C21A—C23A	1.515 (4)
C17—H17	0.9500	C21A—H21C	0.9900
C18—C19	1.393 (4)	C21A—H21D	0.9900
C18—C39	1.524 (5)	C22A—C27A	1.394 (4)
C19—C20	1.392 (4)	C22A—C23A	1.392 (4)
C19—H19	0.9500	C23A—C24A	1.387 (4)
C20—C21	1.520 (4)	C24A—C25A	1.386 (5)
C21—C23	1.523 (4)	C24A—H24A	0.9500
C21—H21A	0.9900	C25A—C26A	1.396 (5)
C21—H21B	0.9900	C25A—C44A	1.533 (4)
C22—C23	1.387 (4)	C26A—C27A	1.394 (4)
C22—C27	1.391 (4)	C26A—H26A	0.9500
C23—C24	1.389 (4)	C27A—C28A	1.520 (4)
C24—C25	1.397 (5)	C28A—H28C	0.9900
C24—H24	0.9500	C28A—H28D	0.9900
C25—C26	1.394 (5)	C29A—C32A	1.517 (5)
C25—C44	1.535 (5)	C29A—C30A	1.528 (5)
C26—C27	1.393 (4)	C29A—C31A	1.540 (5)
C26—H26	0.9500	C30A—H30D	0.9800
C27—C28	1.514 (4)	C30A—H30E	0.9800
C28—H28A	0.9900	C30A—H30F	0.9800
C28—H28B	0.9900	C31A—H31D	0.9800
C29—C32	1.505 (5)	C31A—H31E	0.9800
C29—C30	1.518 (6)	C31A—H31F	0.9800
C29—C31	1.534 (6)	C32A—H32D	0.9800
C30—H30A	0.9800	C32A—H32E	0.9800
C30—H30B	0.9800	C32A—H32F	0.9800
C30—H30C	0.9800	C33A—H33D	0.9800
C31—H31A	0.9800	C33A—H33E	0.9800
C31—H31B	0.9800	C33A—H33F	0.9800

C31—H31C	0.9800	C34A—C35A	1.523 (5)
C32—H32A	0.9800	C34A—C37A	1.529 (5)
C32—H32B	0.9800	C34A—C36A	1.535 (5)
C32—H32C	0.9800	C35A—H35G	0.9800
C33—H33A	0.9800	C35A—H35H	0.9800
C33—H33B	0.9800	C35A—H35I	0.9800
C33—H33C	0.9800	C36A—H36G	0.9800
C34—C36B	1.512 (9)	C36A—H36H	0.9800
C34—C35	1.509 (6)	C36A—H36I	0.9800
C34—C37	1.526 (6)	C37A—H37G	0.9800
C34—C35B	1.545 (10)	C37A—H37H	0.9800
C34—C36	1.556 (6)	C37A—H37I	0.9800
C34—C37B	1.567 (9)	C38A—H38D	0.9800
C35—H35A	0.9800	C38A—H38E	0.9800
C35—H35B	0.9800	C38A—H38F	0.9800
C35—H35C	0.9800	C39A—C42A	1.521 (6)
C36—H36A	0.9800	C39A—C41C	1.524 (10)
C36—H36B	0.9800	C39A—C40A	1.525 (6)
C36—H36C	0.9800	C39A—C41A	1.528 (6)
C37—H37A	0.9800	C39A—C42C	1.530 (10)
C37—H37B	0.9800	C39A—C40C	1.534 (10)
C37—H37C	0.9800	C40A—H40G	0.9800
C35B—H35D	0.9800	C40A—H40H	0.9800
C35B—H35E	0.9800	C40A—H40I	0.9800
C35B—H35F	0.9800	C41A—H41G	0.9800
C36B—H36D	0.9800	C41A—H41H	0.9800
C36B—H36E	0.9800	C41A—H41I	0.9800
C36B—H36F	0.9800	C42A—H42G	0.9800
C37B—H37D	0.9800	C42A—H42H	0.9800
C37B—H37E	0.9800	C42A—H42I	0.9800
C37B—H37F	0.9800	C40C—H40J	0.9800
C38—H38A	0.9800	C40C—H40K	0.9800
C38—H38B	0.9800	C40C—H40L	0.9800
C38—H38C	0.9800	C41C—H41J	0.9800
C39—C41B	1.498 (9)	C41C—H41K	0.9800
C39—C40	1.501 (6)	C41C—H41L	0.9800
C39—C41	1.522 (6)	C42C—H42J	0.9800
C39—C42B	1.537 (9)	C42C—H42K	0.9800
C39—C42	1.547 (6)	C42C—H42L	0.9800
C39—C40B	1.567 (9)	C43A—H43D	0.9800
C40—H40A	0.9800	C43A—H43E	0.9800
C40—H40B	0.9800	C43A—H43F	0.9800
C40—H40C	0.9800	C44A—C46C	1.493 (9)
C41—H41A	0.9800	C44A—C45A	1.501 (6)
C41—H41B	0.9800	C44A—C47A	1.500 (6)
C41—H41C	0.9800	C44A—C47C	1.511 (9)
C42—H42A	0.9800	C44A—C46A	1.596 (6)
C42—H42B	0.9800	C44A—C45C	1.605 (9)
C42—H42C	0.9800	C45A—H45G	0.9800

C40B—H40D	0.9800	C45A—H45H	0.9800
C40B—H40E	0.9800	C45A—H45I	0.9800
C40B—H40F	0.9800	C46A—H46G	0.9800
C41B—H41D	0.9800	C46A—H46H	0.9800
C41B—H41E	0.9800	C46A—H46I	0.9800
C41B—H41F	0.9800	C47A—H47G	0.9800
C42B—H42D	0.9800	C47A—H47H	0.9800
C42B—H42E	0.9800	C47A—H47I	0.9800
C42B—H42F	0.9800	C45C—H45J	0.9800
C43—H43A	0.9800	C45C—H45K	0.9800
C43—H43B	0.9800	C45C—H45L	0.9800
C43—H43C	0.9800	C46C—H46J	0.9800
C44—C47	1.523 (6)	C46C—H46K	0.9800
C44—C45	1.526 (6)	C46C—H46L	0.9800
C44—C46B	1.534 (9)	C47C—H47J	0.9800
C44—C45B	1.537 (10)	C47C—H47K	0.9800
C44—C47B	1.549 (10)	C47C—H47L	0.9800
C44—C46	1.549 (6)	C48A—H48D	0.9800
C45—H45A	0.9800	C48A—H48E	0.9800
C45—H45B	0.9800	C48A—H48F	0.9800
C45—H45C	0.9800	O1H—C4H	1.322 (10)
C46—H46A	0.9800	O1H—C1H	1.420 (12)
C46—H46B	0.9800	C1H—C2H	1.371 (13)
C46—H46C	0.9800	C1H—H1H1	0.9900
C47—H47A	0.9800	C1H—H1H2	0.9900
C47—H47B	0.9800	C2H—C3H	1.363 (11)
C47—H47C	0.9800	C2H—H2H1	0.9900
C45B—H45D	0.9800	C2H—H2H2	0.9900
C45B—H45E	0.9800	C3H—C4H	1.378 (9)
C45B—H45F	0.9800	C3H—H3H1	0.9900
C46B—H46D	0.9800	C3H—H3H2	0.9900
C46B—H46E	0.9800	C4H—H4H1	0.9900
C46B—H46F	0.9800	C4H—H4H2	0.9900
C47B—H47D	0.9800	O1G—C1G	1.455 (7)
C47B—H47E	0.9800	O1G—C4G	1.468 (7)
C47B—H47F	0.9800	C1G—C2G	1.494 (8)
C48—H48A	0.9800	C1G—H1G1	0.9900
C48—H48B	0.9800	C1G—H1G2	0.9900
C48—H48C	0.9800	C2G—C3G	1.512 (9)
O1A—C1A	1.391 (3)	C2G—H2G1	0.9900
O1A—C33A	1.431 (4)	C2G—H2G2	0.9900
O2A—C8A	1.386 (3)	C3G—C4G	1.521 (9)
O2A—C38A	1.424 (3)	C3G—H3G1	0.9900
O3A—C15A	1.395 (3)	C3G—H3G2	0.9900
O3A—C43A	1.431 (4)	C4G—H4G1	0.9900
O4A—C22A	1.392 (3)	C4G—H4G2	0.9900
C1—O1—C33	113.3 (2)	C5A—C4A—C3A	116.5 (3)
C8—O2—C38	115.0 (2)	C5A—C4A—C29A	122.1 (3)
C15—O3—C43	113.5 (2)	C3A—C4A—C29A	121.4 (3)

supplementary materials

C22—O4—C48	113.3 (3)	C4A—C5A—C6A	122.6 (3)
C2—C1—O1	119.3 (3)	C4A—C5A—H5A	118.7
C2—C1—C6	121.1 (3)	C6A—C5A—H5A	118.7
O1—C1—C6	119.5 (3)	C1A—C6A—C5A	118.3 (3)
C1—C2—C3	118.4 (3)	C1A—C6A—C7A	122.1 (3)
C1—C2—C28	120.7 (3)	C5A—C6A—C7A	119.4 (3)
C3—C2—C28	120.7 (3)	C9A—C7A—C6A	111.2 (2)
C2—C3—C4	122.9 (3)	C9A—C7A—H7A1	109.4
C2—C3—H3	118.6	C6A—C7A—H7A1	109.4
C4—C3—H3	118.6	C9A—C7A—H7A2	109.4
C5—C4—C3	116.5 (3)	C6A—C7A—H7A2	109.4
C5—C4—C29	121.4 (3)	H7A1—C7A—H7A2	108.0
C3—C4—C29	122.1 (3)	O2A—C8A—C9A	118.9 (3)
C6—C5—C4	122.8 (3)	O2A—C8A—C13A	119.3 (3)
C6—C5—H5	118.6	C9A—C8A—C13A	121.5 (3)
C4—C5—H5	118.6	C8A—C9A—C10A	118.1 (3)
C5—C6—C1	118.1 (3)	C8A—C9A—C7A	120.9 (3)
C5—C6—C7	119.5 (3)	C10A—C9A—C7A	120.9 (3)
C1—C6—C7	122.3 (3)	C11A—C10A—C9A	122.7 (3)
C6—C7—C9	112.3 (3)	C11A—C10A—H10A	118.7
C6—C7—H7A	109.1	C9A—C10A—H10A	118.7
C9—C7—H7A	109.1	C10A—C11A—C12A	117.0 (3)
C6—C7—H7B	109.1	C10A—C11A—C34A	123.1 (3)
C9—C7—H7B	109.1	C12A—C11A—C34A	120.0 (3)
H7A—C7—H7B	107.9	C13A—C12A—C11A	122.5 (3)
C13—C8—C9	121.7 (3)	C13A—C12A—H12A	118.8
C13—C8—O2	119.4 (3)	C11A—C12A—H12A	118.8
C9—C8—O2	118.7 (3)	C8A—C13A—C12A	118.3 (3)
C8—C9—C10	117.9 (3)	C8A—C13A—C14A	120.7 (3)
C8—C9—C7	120.5 (3)	C12A—C13A—C14A	120.9 (3)
C10—C9—C7	121.5 (3)	C13A—C14A—C16A	110.9 (2)
C11—C10—C9	122.3 (3)	C13A—C14A—H14C	109.5
C11—C10—H10	118.9	C16A—C14A—H14C	109.5
C9—C10—H10	118.9	C13A—C14A—H14D	109.5
C12—C11—C10	117.3 (3)	C16A—C14A—H14D	109.5
C12—C11—C34	121.5 (3)	H14C—C14A—H14D	108.0
C10—C11—C34	121.2 (3)	C16A—C15A—O3A	120.0 (3)
C11—C12—C13	122.6 (3)	C16A—C15A—C20A	120.9 (3)
C11—C12—H12	118.7	O3A—C15A—C20A	119.0 (3)
C13—C12—H12	118.7	C15A—C16A—C17A	118.5 (3)
C8—C13—C12	118.2 (3)	C15A—C16A—C14A	121.4 (3)
C8—C13—C14	120.5 (3)	C17A—C16A—C14A	120.0 (3)
C12—C13—C14	121.2 (3)	C16A—C17A—C18A	122.3 (3)
C16—C14—C13	111.0 (3)	C16A—C17A—H17A	118.9
C16—C14—H14A	109.4	C18A—C17A—H17A	118.9
C13—C14—H14A	109.4	C19A—C18A—C17A	117.3 (3)
C16—C14—H14B	109.4	C19A—C18A—C39A	122.0 (3)
C13—C14—H14B	109.4	C17A—C18A—C39A	120.7 (3)
H14A—C14—H14B	108.0	C18A—C19A—C20A	122.5 (3)

C16—C15—O3	120.0 (3)	C18A—C19A—H19A	118.7
C16—C15—C20	121.1 (3)	C20A—C19A—H19A	118.7
O3—C15—C20	118.8 (3)	C19A—C20A—C15A	118.4 (3)
C15—C16—C17	118.5 (3)	C19A—C20A—C21A	120.7 (3)
C15—C16—C14	121.1 (3)	C15—C20A—C21A	120.9 (3)
C17—C16—C14	120.3 (3)	C23A—C21A—C20A	113.6 (3)
C16—C17—C18	122.8 (3)	C23A—C21A—H21C	108.8
C16—C17—H17	118.6	C20A—C21A—H21C	108.8
C18—C17—H17	118.6	C23A—C21A—H21D	108.8
C17—C18—C19	116.7 (3)	C20A—C21A—H21D	108.8
C17—C18—C39	121.0 (3)	H21C—C21A—H21D	107.7
C19—C18—C39	122.3 (3)	C27A—C22A—O4A	118.8 (3)
C20—C19—C18	122.8 (3)	C27A—C22A—C23A	121.5 (3)
C20—C19—H19	118.6	O4A—C22A—C23A	119.6 (3)
C18—C19—H19	118.6	C24A—C23A—C22A	118.2 (3)
C19—C20—C15	117.9 (3)	C24A—C23A—C21A	120.2 (3)
C19—C20—C21	120.6 (3)	C22A—C23A—C21A	121.5 (3)
C15—C20—C21	121.5 (3)	C25A—C24A—C23A	122.7 (3)
C23—C21—C20	113.7 (3)	C25A—C24A—H24A	118.6
C23—C21—H21A	108.8	C23A—C24A—H24A	118.6
C20—C21—H21A	108.8	C24A—C25A—C26A	117.2 (3)
C23—C21—H21B	108.8	C24A—C25A—C44A	121.9 (3)
C20—C21—H21B	108.8	C26A—C25A—C44A	120.8 (3)
H21A—C21—H21B	107.7	C27A—C26A—C25A	122.3 (3)
C23—C22—C27	122.1 (3)	C27A—C26A—H26A	118.8
C23—C22—O4	119.1 (3)	C25A—C26A—H26A	118.8
C27—C22—O4	118.7 (3)	C22A—C27A—C26A	118.0 (3)
C22—C23—C24	117.9 (3)	C22A—C27A—C28A	121.6 (3)
C22—C23—C21	121.4 (3)	C26A—C27A—C28A	120.4 (3)
C24—C23—C21	120.6 (3)	C27A—C28A—C2A	114.1 (2)
C23—C24—C25	122.5 (3)	C27A—C28A—H28C	108.7
C23—C24—H24	118.8	C2A—C28A—H28C	108.7
C25—C24—H24	118.8	C27A—C28A—H28D	108.7
C26—C25—C24	117.2 (3)	C2A—C28A—H28D	108.7
C26—C25—C44	122.2 (3)	H28C—C28A—H28D	107.6
C24—C25—C44	120.6 (3)	C32A—C29A—C30A	109.8 (4)
C25—C26—C27	122.4 (3)	C32A—C29A—C31A	108.0 (3)
C25—C26—H26	118.8	C30A—C29A—C31A	108.3 (4)
C27—C26—H26	118.8	C32A—C29A—C4A	111.5 (3)
C22—C27—C26	117.8 (3)	C30A—C29A—C4A	110.5 (3)
C22—C27—C28	121.5 (3)	C31A—C29A—C4A	108.6 (3)
C26—C27—C28	120.6 (3)	C29A—C30A—H30D	109.5
C27—C28—C2	112.8 (3)	C29A—C30A—H30E	109.5
C27—C28—H28A	109.0	H30D—C30A—H30E	109.5
C2—C28—H28A	109.0	C29A—C30A—H30F	109.5
C27—C28—H28B	109.0	H30D—C30A—H30F	109.5
C2—C28—H28B	109.0	H30E—C30A—H30F	109.5
H28A—C28—H28B	107.8	C29A—C31A—H31D	109.5
C32—C29—C30	108.5 (4)	C29A—C31A—H31E	109.5

C32—C29—C4	112.2 (3)	H31D—C31A—H31E	109.5
C30—C29—C4	111.8 (3)	C29A—C31A—H31F	109.5
C32—C29—C31	109.2 (4)	H31D—C31A—H31F	109.5
C30—C29—C31	106.8 (4)	H31E—C31A—H31F	109.5
C4—C29—C31	108.2 (3)	C29A—C32A—H32D	109.5
C29—C30—H30A	109.5	C29A—C32A—H32E	109.5
C29—C30—H30B	109.5	H32D—C32A—H32E	109.5
H30A—C30—H30B	109.5	C29A—C32A—H32F	109.5
C29—C30—H30C	109.5	H32D—C32A—H32F	109.5
H30A—C30—H30C	109.5	H32E—C32A—H32F	109.5
H30B—C30—H30C	109.5	O1A—C33A—H33D	109.5
C29—C31—H31A	109.5	O1A—C33A—H33E	109.5
C29—C31—H31B	109.5	H33D—C33A—H33E	109.5
H31A—C31—H31B	109.5	O1A—C33A—H33F	109.5
C29—C31—H31C	109.5	H33D—C33A—H33F	109.5
H31A—C31—H31C	109.5	H33E—C33A—H33F	109.5
H31B—C31—H31C	109.5	C35A—C34A—C37A	109.7 (3)
C29—C32—H32A	109.5	C35A—C34A—C36A	108.8 (3)
C29—C32—H32B	109.5	C37A—C34A—C36A	107.5 (3)
H32A—C32—H32B	109.5	C35A—C34A—C11A	108.8 (3)
C29—C32—H32C	109.5	C37A—C34A—C11A	109.9 (3)
H32A—C32—H32C	109.5	C36A—C34A—C11A	112.2 (3)
H32B—C32—H32C	109.5	C34A—C35A—H35G	109.5
O1—C33—H33A	109.5	C34A—C35A—H35H	109.5
O1—C33—H33B	109.5	H35G—C35A—H35H	109.5
H33A—C33—H33B	109.5	C34A—C35A—H35I	109.5
O1—C33—H33C	109.5	H35G—C35A—H35I	109.5
H33A—C33—H33C	109.5	H35H—C35A—H35I	109.5
H33B—C33—H33C	109.5	C34A—C36A—H36G	109.5
C36B—C34—C35	138.1 (7)	C34A—C36A—H36H	109.5
C36B—C34—C37	51.0 (9)	H36G—C36A—H36H	109.5
C35—C34—C37	114.3 (6)	C34A—C36A—H36I	109.5
C36B—C34—C11	113.0 (7)	H36G—C36A—H36I	109.5
C35—C34—C11	108.9 (4)	H36H—C36A—H36I	109.5
C37—C34—C11	107.5 (4)	C34A—C37A—H37G	109.5
C36B—C34—C35B	109.9 (12)	C34A—C37A—H37H	109.5
C35—C34—C35B	55.2 (8)	H37G—C37A—H37H	109.5
C37—C34—C35B	143.1 (8)	C34A—C37A—H37I	109.5
C11—C34—C35B	109.3 (7)	H37G—C37A—H37I	109.5
C36B—C34—C36	57.6 (10)	H37H—C37A—H37I	109.5
C35—C34—C36	107.5 (5)	O2A—C38A—H38D	109.5
C37—C34—C36	107.0 (5)	O2A—C38A—H38E	109.5
C11—C34—C36	111.7 (4)	H38D—C38A—H38E	109.5
C35B—C34—C36	55.8 (8)	O2A—C38A—H38F	109.5
C36B—C34—C37B	107.6 (12)	H38D—C38A—H38F	109.5
C35—C34—C37B	52.3 (9)	H38E—C38A—H38F	109.5
C37—C34—C37B	63.6 (9)	C42A—C39A—C41C	61.7 (11)
C11—C34—C37B	112.9 (7)	C42A—C39A—C40A	118.3 (6)
C35B—C34—C37B	103.7 (12)	C41C—C39A—C40A	130.7 (9)

C36—C34—C37B	135.0 (8)	C42A—C39A—C41A	106.7 (6)
C34—C35—H35A	109.5	C41C—C39A—C41A	47.1 (10)
C34—C35—H35B	109.5	C40A—C39A—C41A	98.4 (6)
C34—C35—H35C	109.5	C42A—C39A—C42C	41.3 (14)
C34—C36—H36A	109.5	C41C—C39A—C42C	101.8 (17)
C34—C36—H36B	109.5	C40A—C39A—C42C	85.7 (16)
C34—C36—H36C	109.5	C41A—C39A—C42C	140.5 (13)
C34—C37—H37A	109.5	C42A—C39A—C40C	85.8 (15)
C34—C37—H37B	109.5	C41C—C39A—C40C	135.0 (15)
C34—C37—H37C	109.5	C40A—C39A—C40C	39.9 (12)
C34—C35B—H35D	109.5	C41A—C39A—C40C	132.9 (12)
C34—C35B—H35E	109.5	C42C—C39A—C40C	47.1 (18)
H35D—C35B—H35E	109.5	C42A—C39A—C18A	110.8 (4)
C34—C35B—H35F	109.5	C41C—C39A—C18A	111.4 (9)
H35D—C35B—H35F	109.5	C40A—C39A—C18A	112.9 (3)
H35E—C35B—H35F	109.5	C41A—C39A—C18A	108.4 (3)
C34—C36B—H36D	109.5	C42C—C39A—C18A	106.0 (12)
C34—C36B—H36E	109.5	C40C—C39A—C18A	108.8 (9)
H36D—C36B—H36E	109.5	C39A—C40A—H40G	109.5
C34—C36B—H36F	109.5	C39A—C40A—H40H	109.5
H36D—C36B—H36F	109.5	C39A—C40A—H40I	109.5
H36E—C36B—H36F	109.5	C39A—C41A—H41G	109.5
C34—C37B—H37D	109.5	C39A—C41A—H41H	109.5
C34—C37B—H37E	109.5	C39A—C41A—H41I	109.5
H37D—C37B—H37E	109.5	C39A—C42A—H42G	109.5
C34—C37B—H37F	109.5	C39A—C42A—H42H	109.5
H37D—C37B—H37F	109.5	C39A—C42A—H42I	109.5
H37E—C37B—H37F	109.5	C39A—C40C—H40J	109.5
O2—C38—H38A	109.5	C39A—C40C—H40K	109.5
O2—C38—H38B	109.5	H40J—C40C—H40K	109.5
H38A—C38—H38B	109.5	C39A—C40C—H40L	109.5
O2—C38—H38C	109.5	H40J—C40C—H40L	109.5
H38A—C38—H38C	109.5	H40K—C40C—H40L	109.5
H38B—C38—H38C	109.5	C39A—C41C—H41J	109.5
C41B—C39—C40	129.2 (8)	C39A—C41C—H41K	109.5
C41B—C39—C41	48.0 (9)	H41J—C41C—H41K	109.5
C40—C39—C41	110.0 (5)	C39A—C41C—H41L	109.5
C41B—C39—C18	115.6 (8)	H41J—C41C—H41L	109.5
C40—C39—C18	115.1 (3)	H41K—C41C—H41L	109.5
C41—C39—C18	109.9 (4)	C39A—C42C—H42J	109.5
C41B—C39—C42B	115.3 (12)	C39A—C42C—H42K	109.5
C40—C39—C42B	48.7 (8)	H42J—C42C—H42K	109.5
C41—C39—C42B	141.8 (8)	C39A—C42C—H42L	109.5
C18—C39—C42B	108.3 (7)	H42J—C42C—H42L	109.5
C41B—C39—C42	58.3 (9)	H42K—C42C—H42L	109.5
C40—C39—C42	107.1 (5)	O3A—C43A—H43D	109.5
C41—C39—C42	105.6 (5)	O3A—C43A—H43E	109.5
C18—C39—C42	108.7 (4)	H43D—C43A—H43E	109.5
C42B—C39—C42	64.0 (8)	O3A—C43A—H43F	109.5

C41B—C39—C40B	111.4 (11)	H43D—C43A—H43F	109.5
C40—C39—C40B	52.1 (7)	H43E—C43A—H43F	109.5
C41—C39—C40B	67.2 (7)	C46C—C44A—C45A	48.5 (7)
C18—C39—C40B	103.9 (6)	C46C—C44A—C47A	138.4 (6)
C42B—C39—C40B	100.8 (10)	C45A—C44A—C47A	120.1 (6)
C42—C39—C40B	146.9 (7)	C46C—C44A—C47C	116.8 (10)
C39—C40—H40A	109.5	C45A—C44A—C47C	140.4 (8)
C39—C40—H40B	109.5	C47A—C44A—C47C	40.4 (7)
C39—C40—H40C	109.5	C46C—C44A—C25A	111.1 (6)
C39—C41—H41A	109.5	C45A—C44A—C25A	110.4 (3)
C39—C41—H41B	109.5	C47A—C44A—C25A	110.0 (4)
C39—C41—H41C	109.5	C47C—C44A—C25A	109.2 (7)
C39—C42—H42A	109.5	C46C—C44A—C46A	54.5 (7)
C39—C42—H42B	109.5	C45A—C44A—C46A	101.0 (5)
C39—C42—H42C	109.5	C47A—C44A—C46A	104.6 (6)
C39—C40B—H40D	109.5	C47C—C44A—C46A	67.0 (8)
C39—C40B—H40E	109.5	C25A—C44A—C46A	109.9 (3)
H40D—C40B—H40E	109.5	C46C—C44A—C45C	103.3 (9)
C39—C40B—H40F	109.5	C45A—C44A—C45C	58.1 (6)
H40D—C40B—H40F	109.5	C47A—C44A—C45C	66.8 (7)
H40E—C40B—H40F	109.5	C47C—C44A—C45C	104.5 (9)
C39—C41B—H41D	109.5	C25A—C44A—C45C	111.6 (5)
C39—C41B—H41E	109.5	C46A—C44A—C45C	137.9 (5)
H41D—C41B—H41E	109.5	C44A—C45A—H45G	109.5
C39—C41B—H41F	109.5	C44A—C45A—H45H	109.5
H41D—C41B—H41F	109.5	C44A—C45A—H45I	109.5
H41E—C41B—H41F	109.5	C44A—C46A—H46G	109.5
C39—C42B—H42D	109.5	C44A—C46A—H46H	109.5
C39—C42B—H42E	109.5	C44A—C46A—H46I	109.5
H42D—C42B—H42E	109.5	C44A—C47A—H47G	109.5
C39—C42B—H42F	109.5	C44A—C47A—H47H	109.5
H42D—C42B—H42F	109.5	C44A—C47A—H47I	109.5
H42E—C42B—H42F	109.5	C44A—C45C—H45J	109.5
O3—C43—H43A	109.5	C44A—C45C—H45K	109.5
O3—C43—H43B	109.5	H45J—C45C—H45K	109.5
H43A—C43—H43B	109.5	C44A—C45C—H45L	109.5
O3—C43—H43C	109.5	H45J—C45C—H45L	109.5
H43A—C43—H43C	109.5	H45K—C45C—H45L	109.5
H43B—C43—H43C	109.5	C44A—C46C—H46J	109.5
C47—C44—C45	108.8 (5)	C44A—C46C—H46K	109.5
C47—C44—C46B	64.3 (12)	H46J—C46C—H46K	109.5
C45—C44—C46B	139.5 (9)	C44A—C46C—H46L	109.5
C47—C44—C25	113.2 (4)	H46J—C46C—H46L	109.5
C45—C44—C25	110.1 (4)	H46K—C46C—H46L	109.5
C46B—C44—C25	108.8 (9)	C44A—C47C—H47J	109.5
C47—C44—C45B	130.8 (10)	C44A—C47C—H47K	109.5
C45—C44—C45B	42.4 (10)	H47J—C47C—H47K	109.5
C46B—C44—C45B	109.4 (13)	C44A—C47C—H47L	109.5
C25—C44—C45B	114.6 (9)	H47J—C47C—H47L	109.5

C47—C44—C47B	46.3 (8)	H47K—C47C—H47L	109.5
C45—C44—C47B	68.6 (10)	O4A—C48A—H48D	109.5
C46B—C44—C47B	109.8 (14)	O4A—C48A—H48E	109.5
C25—C44—C47B	107.0 (8)	H48D—C48A—H48E	109.5
C45B—C44—C47B	107.2 (14)	O4A—C48A—H48F	109.5
C47—C44—C46	109.2 (5)	H48D—C48A—H48F	109.5
C45—C44—C46	107.8 (5)	H48E—C48A—H48F	109.5
C46B—C44—C46	48.6 (11)	C4H—O1H—C1H	108.5 (10)
C25—C44—C46	107.6 (4)	C2H—C1H—O1H	103.1 (8)
C45B—C44—C46	66.3 (11)	C2H—C1H—H1H1	111.1
C47B—C44—C46	144.0 (8)	O1H—C1H—H1H1	111.1
C44—C45—H45A	109.5	C2H—C1H—H1H2	111.1
C44—C45—H45B	109.5	O1H—C1H—H1H2	111.1
C44—C45—H45C	109.5	H1H1—C1H—H1H2	109.1
C44—C46—H46A	109.5	C3H—C2H—C1H	111.0 (10)
C44—C46—H46B	109.5	C3H—C2H—H2H1	109.4
C44—C46—H46C	109.5	C1H—C2H—H2H1	109.4
C44—C47—H47A	109.5	C3H—C2H—H2H2	109.4
C44—C47—H47B	109.5	C1H—C2H—H2H2	109.4
C44—C47—H47C	109.5	H2H1—C2H—H2H2	108.0
C44—C45B—H45D	109.5	C2H—C3H—C4H	105.6 (8)
C44—C45B—H45E	109.5	C2H—C3H—H3H1	110.6
H45D—C45B—H45E	109.5	C4H—C3H—H3H1	110.6
C44—C45B—H45F	109.5	C2H—C3H—H3H2	110.6
H45D—C45B—H45F	109.5	C4H—C3H—H3H2	110.6
H45E—C45B—H45F	109.5	H3H1—C3H—H3H2	108.8
C44—C46B—H46D	109.5	O1H—C4H—C3H	109.2 (9)
C44—C46B—H46E	109.5	O1H—C4H—H4H1	109.8
H46D—C46B—H46E	109.5	C3H—C4H—H4H1	109.8
C44—C46B—H46F	109.5	O1H—C4H—H4H2	109.8
H46D—C46B—H46F	109.5	C3H—C4H—H4H2	109.8
H46E—C46B—H46F	109.5	H4H1—C4H—H4H2	108.3
C44—C47B—H47D	109.5	C1G—O1G—C4G	103.3 (8)
C44—C47B—H47E	109.5	O1G—C1G—C2G	103.4 (9)
H47D—C47B—H47E	109.5	O1G—C1G—H1G1	111.1
C44—C47B—H47F	109.5	C2G—C1G—H1G1	111.1
H47D—C47B—H47F	109.5	O1G—C1G—H1G2	111.1
H47E—C47B—H47F	109.5	C2G—C1G—H1G2	111.1
O4—C48—H48A	109.5	H1G1—C1G—H1G2	109.1
O4—C48—H48B	109.5	C1G—C2G—C3G	115.4 (11)
H48A—C48—H48B	109.5	C1G—C2G—H2G1	108.4
O4—C48—H48C	109.5	C3G—C2G—H2G1	108.4
H48A—C48—H48C	109.5	C1G—C2G—H2G2	108.4
H48B—C48—H48C	109.5	C3G—C2G—H2G2	108.4
C1A—O1A—C33A	113.9 (2)	H2G1—C2G—H2G2	107.5
C8A—O2A—C38A	115.7 (2)	C2G—C3G—C4G	90.6 (8)
C15A—O3A—C43A	113.6 (2)	C2G—C3G—H3G1	113.5
C22A—O4A—C48A	115.4 (2)	C4G—C3G—H3G1	113.5
C2A—C1A—O1A	119.5 (3)	C2G—C3G—H3G2	113.5

C2A—C1A—C6A	120.7 (3)	C4G—C3G—H3G2	113.5
O1A—C1A—C6A	119.7 (3)	H3G1—C3G—H3G2	110.8
C3A—C2A—C1A	118.8 (3)	O1G—C4G—C3G	113.6 (9)
C3A—C2A—C28A	120.2 (3)	O1G—C4G—H4G1	108.8
C1A—C2A—C28A	120.9 (3)	C3G—C4G—H4G1	108.8
C2A—C3A—C4A	123.0 (3)	O1G—C4G—H4G2	108.8
C2A—C3A—H3A	118.5	C3G—C4G—H4G2	108.8
C4A—C3A—H3A	118.5	H4G1—C4G—H4G2	107.7
C33—O1—C1—C2	−91.3 (3)	O1A—C1A—C2A—C3A	−179.7 (3)
C33—O1—C1—C6	93.2 (3)	C6A—C1A—C2A—C3A	−3.9 (4)
O1—C1—C2—C3	179.5 (3)	O1A—C1A—C2A—C28A	−3.5 (4)
C6—C1—C2—C3	−5.1 (5)	C6A—C1A—C2A—C28A	172.4 (3)
O1—C1—C2—C28	−4.5 (4)	C1A—C2A—C3A—C4A	1.6 (5)
C6—C1—C2—C28	170.9 (3)	C28A—C2A—C3A—C4A	−174.7 (3)
C1—C2—C3—C4	2.6 (5)	C2A—C3A—C4A—C5A	1.2 (4)
C28—C2—C3—C4	−173.4 (3)	C2A—C3A—C4A—C29A	179.6 (3)
C2—C3—C4—C5	0.3 (5)	C3A—C4A—C5A—C6A	−1.9 (4)
C2—C3—C4—C29	−178.6 (3)	C29A—C4A—C5A—C6A	179.8 (3)
C3—C4—C5—C6	−0.9 (5)	C2A—C1A—C6A—C5A	3.2 (4)
C29—C4—C5—C6	178.0 (3)	O1A—C1A—C6A—C5A	179.1 (3)
C4—C5—C6—C1	−1.5 (5)	C2A—C1A—C6A—C7A	−172.1 (3)
C4—C5—C6—C7	175.9 (3)	O1A—C1A—C6A—C7A	3.7 (4)
C2—C1—C6—C5	4.5 (5)	C4A—C5A—C6A—C1A	−0.3 (4)
O1—C1—C6—C5	180.0 (3)	C4A—C5A—C6A—C7A	175.2 (3)
C2—C1—C6—C7	−172.7 (3)	C1A—C6A—C7A—C9A	111.1 (3)
O1—C1—C6—C7	2.7 (4)	C5A—C6A—C7A—C9A	−64.2 (3)
C5—C6—C7—C9	−63.0 (4)	C38A—O2A—C8A—C9A	−94.7 (3)
C1—C6—C7—C9	114.3 (3)	C38A—O2A—C8A—C13A	90.8 (3)
C38—O2—C8—C13	90.6 (3)	O2A—C8A—C9A—C10A	−174.6 (2)
C38—O2—C8—C9	−93.7 (3)	C13A—C8A—C9A—C10A	−0.3 (4)
C13—C8—C9—C10	−0.2 (5)	O2A—C8A—C9A—C7A	2.9 (4)
O2—C8—C9—C10	−175.8 (3)	C13A—C8A—C9A—C7A	177.3 (3)
C13—C8—C9—C7	177.5 (3)	C6A—C7A—C9A—C8A	−69.8 (3)
O2—C8—C9—C7	2.0 (4)	C6A—C7A—C9A—C10A	107.7 (3)
C6—C7—C9—C8	−66.9 (4)	C8A—C9A—C10A—C11A	0.3 (4)
C6—C7—C9—C10	110.7 (3)	C7A—C9A—C10A—C11A	−177.3 (3)
C8—C9—C10—C11	−0.6 (5)	C9A—C10A—C11A—C12A	−1.1 (4)
C7—C9—C10—C11	−178.3 (3)	C9A—C10A—C11A—C34A	177.6 (3)
C9—C10—C11—C12	0.9 (5)	C10A—C11A—C12A—C13A	2.0 (4)
C9—C10—C11—C34	179.8 (3)	C34A—C11A—C12A—C13A	−176.7 (3)
C10—C11—C12—C13	−0.4 (5)	O2A—C8A—C13A—C12A	175.4 (2)
C34—C11—C12—C13	−179.3 (3)	C9A—C8A—C13A—C12A	1.1 (4)
C9—C8—C13—C12	0.7 (5)	O2A—C8A—C13A—C14A	0.5 (4)
O2—C8—C13—C12	176.2 (3)	C9A—C8A—C13A—C14A	−173.9 (3)
C9—C8—C13—C14	−174.9 (3)	C11A—C12A—C13A—C8A	−2.1 (4)
O2—C8—C13—C14	0.6 (4)	C11A—C12A—C13A—C14A	172.9 (3)
C11—C12—C13—C8	−0.4 (5)	C8A—C13A—C14A—C16A	69.5 (4)
C11—C12—C13—C14	175.2 (3)	C12A—C13A—C14A—C16A	−105.4 (3)
C8—C13—C14—C16	67.8 (4)	C43A—O3A—C15A—C16A	−92.8 (3)

C12—C13—C14—C16	−107.7 (3)	C43A—O3A—C15A—C20A	90.3 (3)
C43—O3—C15—C16	−92.2 (3)	O3A—C15A—C16A—C17A	−179.3 (2)
C43—O3—C15—C20	90.8 (3)	C20A—C15A—C16A—C17A	−2.4 (4)
O3—C15—C16—C17	179.9 (3)	O3A—C15A—C16A—C14A	−2.6 (4)
C20—C15—C16—C17	−3.2 (5)	C20A—C15A—C16A—C14A	174.2 (3)
O3—C15—C16—C14	−3.3 (4)	C13A—C14A—C16A—C15A	−113.9 (3)
C20—C15—C16—C14	173.6 (3)	C13A—C14A—C16A—C17A	62.7 (4)
C13—C14—C16—C15	−111.7 (3)	C15A—C16A—C17A—C18A	−0.2 (4)
C13—C14—C16—C17	65.1 (4)	C14A—C16A—C17A—C18A	−176.9 (3)
C15—C16—C17—C18	0.4 (5)	C16A—C17A—C18A—C19A	1.6 (5)
C14—C16—C17—C18	−176.5 (3)	C16A—C17A—C18A—C39A	179.3 (3)
C16—C17—C18—C19	2.3 (5)	C17A—C18A—C19A—C20A	−0.6 (5)
C16—C17—C18—C39	−178.8 (3)	C39A—C18A—C19A—C20A	−178.3 (3)
C17—C18—C19—C20	−2.2 (5)	C18A—C19A—C20A—C15A	−1.9 (5)
C39—C18—C19—C20	178.8 (3)	C18A—C19A—C20A—C21A	175.0 (3)
C18—C19—C20—C15	−0.4 (5)	C16A—C15A—C20A—C19A	3.4 (4)
C18—C19—C20—C21	177.7 (3)	O3A—C15A—C20A—C19A	−179.7 (3)
C16—C15—C20—C19	3.2 (4)	C16A—C15A—C20A—C21A	−173.5 (3)
O3—C15—C20—C19	−179.8 (3)	O3A—C15A—C20A—C21A	3.4 (4)
C16—C15—C20—C21	−174.9 (3)	C19A—C20A—C21A—C23A	−117.9 (3)
O3—C15—C20—C21	2.1 (4)	C15A—C20A—C21A—C23A	58.9 (4)
C19—C20—C21—C23	−121.5 (3)	C48A—O4A—C22A—C27A	−95.4 (3)
C15—C20—C21—C23	56.6 (4)	C48A—O4A—C22A—C23A	89.0 (3)
C48—O4—C22—C23	92.1 (4)	C27A—C22A—C23A—C24A	1.6 (4)
C48—O4—C22—C27	−90.5 (3)	O4A—C22A—C23A—C24A	177.1 (3)
C27—C22—C23—C24	3.5 (5)	C27A—C22A—C23A—C21A	−175.2 (3)
O4—C22—C23—C24	−179.2 (3)	O4A—C22A—C23A—C21A	0.3 (4)
C27—C22—C23—C21	−173.3 (3)	C20A—C21A—C23A—C24A	−116.3 (3)
O4—C22—C23—C21	4.0 (4)	C20A—C21A—C23A—C22A	60.5 (4)
C20—C21—C23—C22	67.3 (4)	C22A—C23A—C24A—C25A	−0.6 (5)
C20—C21—C23—C24	−109.4 (3)	C21A—C23A—C24A—C25A	176.3 (3)
C22—C23—C24—C25	−2.0 (5)	C23A—C24A—C25A—C26A	−0.7 (5)
C21—C23—C24—C25	174.8 (3)	C23A—C24A—C25A—C44A	−178.0 (3)
C23—C24—C25—C26	−0.5 (5)	C24A—C25A—C26A—C27A	1.1 (5)
C23—C24—C25—C44	179.6 (3)	C44A—C25A—C26A—C27A	178.4 (3)
C24—C25—C26—C27	1.7 (5)	O4A—C22A—C27A—C26A	−176.8 (3)
C44—C25—C26—C27	−178.5 (3)	C23A—C22A—C27A—C26A	−1.2 (4)
C23—C22—C27—C26	−2.4 (5)	O4A—C22A—C27A—C28A	2.7 (4)
O4—C22—C27—C26	−179.7 (3)	C23A—C22A—C27A—C28A	178.3 (3)
C23—C22—C27—C28	174.4 (3)	C25A—C26A—C27A—C22A	−0.2 (5)
O4—C22—C27—C28	−2.9 (4)	C25A—C26A—C27A—C28A	−179.7 (3)
C25—C26—C27—C22	−0.3 (5)	C22A—C27A—C28A—C2A	−61.6 (4)
C25—C26—C27—C28	−177.2 (3)	C26A—C27A—C28A—C2A	117.9 (3)
C22—C27—C28—C2	−63.3 (4)	C3A—C2A—C28A—C27A	114.3 (3)
C26—C27—C28—C2	113.4 (3)	C1A—C2A—C28A—C27A	−61.9 (4)
C1—C2—C28—C27	−63.4 (4)	C5A—C4A—C29A—C32A	24.7 (4)
C3—C2—C28—C27	112.5 (3)	C3A—C4A—C29A—C32A	−153.6 (3)
C5—C4—C29—C32	31.4 (5)	C5A—C4A—C29A—C30A	147.2 (4)
C3—C4—C29—C32	−149.7 (4)	C3A—C4A—C29A—C30A	−31.1 (5)

supplementary materials

C5—C4—C29—C30	153.6 (4)	C5A—C4A—C29A—C31A	−94.2 (4)	
C3—C4—C29—C30	−27.6 (5)	C3A—C4A—C29A—C31A	87.6 (4)	
C5—C4—C29—C31	−89.1 (4)	C10A—C11A—C34A—C35A	−119.3 (3)	
C3—C4—C29—C31	89.7 (4)	C12A—C11A—C34A—C35A	59.4 (4)	
C12—C11—C34—C36B	−122.7 (12)	C10A—C11A—C34A—C37A	120.7 (3)	
C10—C11—C34—C36B	58.5 (12)	C12A—C11A—C34A—C37A	−60.7 (4)	
C12—C11—C34—C35	55.8 (6)	C10A—C11A—C34A—C36A	1.2 (4)	
C10—C11—C34—C35	−123.0 (6)	C12A—C11A—C34A—C36A	179.8 (3)	
C12—C11—C34—C37	−68.4 (5)	C19A—C18A—C39A—C42A	−132.6 (6)	
C10—C11—C34—C37	112.8 (5)	C17A—C18A—C39A—C42A	49.9 (7)	
C12—C11—C34—C35B	114.5 (9)	C19A—C18A—C39A—C41C	160.8 (12)	
C10—C11—C34—C35B	−64.3 (9)	C17A—C18A—C39A—C41C	−16.8 (13)	
C12—C11—C34—C36	174.5 (4)	C19A—C18A—C39A—C40A	2.8 (6)	
C10—C11—C34—C36	−4.3 (6)	C17A—C18A—C39A—C40A	−174.8 (5)	
C12—C11—C34—C37B	−0.3 (11)	C19A—C18A—C39A—C41A	110.6 (5)	
C10—C11—C34—C37B	−179.1 (11)	C17A—C18A—C39A—C41A	−66.9 (5)	
C17—C18—C39—C41B	−5.8 (12)	C19A—C18A—C39A—C42C	−89.3 (17)	
C19—C18—C39—C41B	173.1 (11)	C17A—C18A—C39A—C42C	93.1 (17)	
C17—C18—C39—C40	177.4 (5)	C19A—C18A—C39A—C40C	−39.9 (15)	
C19—C18—C39—C40	−3.7 (6)	C17A—C18A—C39A—C40C	142.6 (15)	
C17—C18—C39—C41	−57.8 (6)	C24A—C25A—C44A—C46C	−70.2 (8)	
C19—C18—C39—C41	121.1 (5)	C26A—C25A—C44A—C46C	112.7 (8)	
C17—C18—C39—C42B	125.2 (9)	C24A—C25A—C44A—C45A	−122.3 (5)	
C19—C18—C39—C42B	−55.9 (10)	C26A—C25A—C44A—C45A	60.6 (6)	
C17—C18—C39—C42	57.3 (5)	C24A—C25A—C44A—C47A	103.0 (6)	
C19—C18—C39—C42	−123.8 (5)	C26A—C25A—C44A—C47A	−74.2 (6)	
C17—C18—C39—C40B	−128.2 (7)	C24A—C25A—C44A—C47C	60.0 (9)	
C19—C18—C39—C40B	50.7 (8)	C26A—C25A—C44A—C47C	−117.1 (8)	
C26—C25—C44—C47	−7.6 (6)	C24A—C25A—C44A—C46A	−11.7 (5)	
C24—C25—C44—C47	172.2 (5)	C26A—C25A—C44A—C46A	171.2 (4)	
C26—C25—C44—C45	−129.6 (5)	C24A—C25A—C44A—C45C	175.1 (7)	
C24—C25—C44—C45	50.2 (6)	C26A—C25A—C44A—C45C	−2.1 (8)	
C26—C25—C44—C46B	61.8 (14)	C4H—O1H—C1H—C2H	−16.3 (15)	
C24—C25—C44—C46B	−118.4 (13)	O1H—C1H—C2H—C3H	11.8 (17)	
C26—C25—C44—C45B	−175.4 (13)	C1H—C2H—C3H—C4H	−3.4 (15)	
C24—C25—C44—C45B	4.4 (13)	C1H—O1H—C4H—C3H	15.0 (13)	
C26—C25—C44—C47B	−56.8 (11)	C2H—C3H—C4H—O1H	−7.4 (12)	
C24—C25—C44—C47B	123.1 (10)	C4G—O1G—C1G—C2G	−10.7 (12)	
C26—C25—C44—C46	113.2 (5)	O1G—C1G—C2G—C3G	−13.6 (19)	
C24—C25—C44—C46	−67.0 (5)	C1G—C2G—C3G—C4G	29.3 (18)	
C33A—O1A—C1A—C2A	−85.8 (3)	C1G—O1G—C4G—C3G	33.1 (12)	
C33A—O1A—C1A—C6A	98.3 (3)	C2G—C3G—C4G—O1G	−36.9 (14)	

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C14A—H14D⋯CgA[i]	0.99	2.93	3.817	149
C43—H43A⋯CgC	0.98	2.64	3.426	137
C48—H48A⋯CgA[ii]	0.98	2.82	3.586	136

C48A—H48D⋯CgB[ii]   0.98   2.84   3.580   133

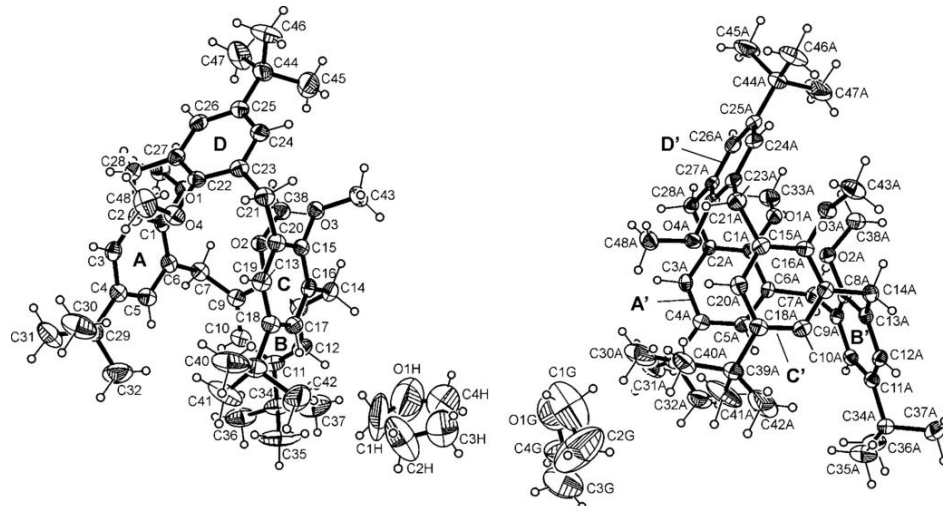Symmetry codes: (i) −x+2, y−1/2, −z+1/2; (ii) −x+1, y+1/2, −z+1/2.

Fig. 1

Fig. 2