

6,12,18,24-Tetramethoxy-4,10,16,22-tetrakis[(methoxycarbonyl)methoxy]-2,8,14,20-tetrakis(2-phenylethyl)-resorcin[4]arene

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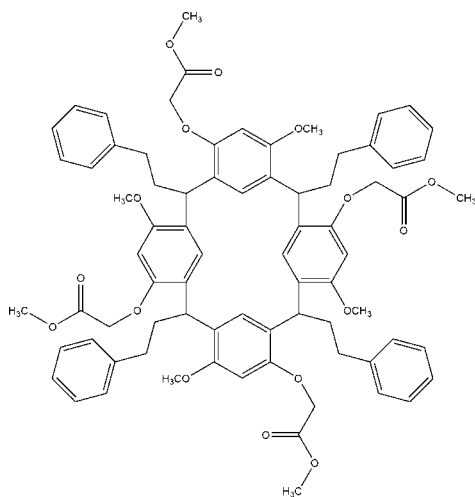
Received 27 October 2011; accepted 30 November 2011

Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.056; wR factor = 0.162; data-to-parameter ratio = 10.0.

The title compound, $\text{C}_{76}\text{H}_{80}\text{O}_{16}$, is a macrocyclic structure. This novel resorcin[4]arene derivative has (methoxycarbonyl)methoxy 'head' groups on the upper rim. The compound has a C_{2v} 'boat' geometry and there are a range of $\text{C}-\text{H}\cdots\text{O}$ contacts in the crystal structure.

Related literature

For applications of resorcin[4]arenes, see: Ajami *et al.* (2011); Sun *et al.* (2010); Arnott *et al.* (2006); Sokoljess *et al.* (2002). For structural information, see: Wiegmann & Mattay (2011); Pansuriya *et al.* (2011). For details of $\text{C}-\text{H}\cdots\pi$ interactions, see: Nishio (2004). For the synthesis of tetramethoxy resorcin[4]arenes: McIldowie *et al.* (2000).



Experimental

Crystal data

$\text{C}_{76}\text{H}_{80}\text{O}_{16}$
 $M_r = 1249.40$
Monoclinic, $P2_1$
 $a = 14.1361$ (7) Å
 $b = 32.2264$ (17) Å
 $c = 28.9417$ (16) Å
 $\beta = 90.572$ (1)°
 $V = 13183.9$ (12) Å³
 $Z = 8$
Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 173$ K
 $0.41 \times 0.33 \times 0.29$ mm

Data collection

Bruker Kappa DUO APEXII diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2006)
 $T_{\min} = 0.965$, $T_{\max} = 0.975$
126671 measured reflections
33391 independent reflections
23289 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.072$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.056$
 $wR(F^2) = 0.162$
 $S = 1.02$
33391 reflections
3345 parameters
1 restraint
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.44$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.33$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C14B}-\text{H14B}\cdots\text{O16A}^i$	1.00	2.59	3.440 (4)	142
$\text{C30B}-\text{H30C}\cdots\text{O11A}^i$	0.99	2.49	3.464 (6)	169
$\text{C30C}-\text{H30F}\cdots\text{O8D}^{ii}$	0.99	2.55	3.259 (4)	128
$\text{C30D}-\text{H30G}\cdots\text{O8C}^{iii}$	0.99	2.56	3.270 (5)	129
$\text{C44A}-\text{H44B}\cdots\text{O10B}^{iv}$	0.98	2.54	3.292 (5)	133
$\text{C56C}-\text{H56H}\cdots\text{O7B}^v$	0.98	2.55	3.375 (9)	141
$\text{C56D}-\text{H56K}\cdots\text{O15A}^{vi}$	0.98	2.37	3.251 (8)	149
$\text{C62C}-\text{H62C}\cdots\text{O7C}^{vii}$	0.95	2.46	3.313 (6)	149
$\text{C62D}-\text{H62D}\cdots\text{O7D}^{viii}$	0.95	2.59	3.421 (7)	146
$\text{C63A}-\text{H63A}\cdots\text{O3B}^{viii}$	0.95	2.37	3.267 (7)	156

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

Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 2006); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: SHELXL97.

The authors wish to thank Dr Hong Su from the Chemistry Department of the University of Cape Town for her assistance with the data collection and refinement and the DST – National Research Foundation Centre of Excellence in Catalysis, c*change for financial support. PBP is thankful to the University of KwaZulu-Natal for a postdoctoral fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5129).

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supplementary materials

Acta Cryst. (2012). E68, o97-o98 [doi:10.1107/S1600536811051567]

6,12,18,24-Tetramethoxy-4,10,16,22-tetrakis[(methoxycarbonyl)methoxy]-2,8,14,20-tetrakis(2-phenylethyl)resorcin[4]arene

P. B. Pansuriya, H. B. Friedrich and G. E. M. Maguire

Comment

Resorcin[4]arene derivatives with different physicochemical properties have received extensive research interest (Ajami *et al.*, 2011; Sun *et al.*, 2010; Arnott *et al.*, 2006; Sokoliess *et al.*, 2002). One such family of relevant molecules that has been reported on is the semi-flexible tetramethoxy resorcin[4]arenes (Wiegmann & Mattay 2011). Here we report the crystal structure of a novel tetramethoxy resorcin[4]arene derivative containing (methoxycarbonyl)methoxy "head" groups on the upper rim.

The title compound is racemic and has an *rccc* (boat) configuration (Fig. 1). This differs from our previously reported octamethoxy resorcin[4]arene structure which had a chair (*rctt*) configuration (Pansuriya *et al.*, 2011). Several non-classical inter- and intramolecular weak hydrogen bonds are present in the structure. C—H \cdots π contacts (Nishio, 2004) involving methoxy, ester groups and neighbouring aromatic rings with H \cdots π distances (centroid of the aromatic ring) ranging from 2.62 to 2.96 Å are present. Interlocking of (methoxycarbonyl)methoxy head groups on the upper rim and interdigitation of the "feet" in lower rim create infinite columns these interactions in [100] plane (Fig. 2).

Experimental

In dry degassed acetonitrile (100 ml) tetramethoxy resorcin[4]arene (0.58 g, 0.6 mmol) and anhydrous potassium carbonate (0.785 g, 5.7 mmol) were added. The reaction was stirred at 70 °C for ten minutes and then methyl acetyl bromide (425 μ l, 4.6 mmol) was added dropwise. The reaction solution was allowed to reflux for 24 h and then cooled to room temperature. The solvent was reduced under vacuum and the resulting residue extracted with DCM (100 ml). The DCM was washed with 1M HCl (50 ml), water (50 ml) and then brine (50 ml). The organic layer was separated and dried over anhydrous magnesium sulfate. The solvent was reduced to complete dryness to afford the product as a white solid (Yield: 0.60 g, 80%), *M.p.* 387 K.

Crystal suitable for X-ray diffraction analysis were grown at room temperature from a solution of DCM:methanol (2:1).

Refinement

All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed at calculated positions with attach distances ranging from 0.95 Å to 1.00 Å and refined as riding on their parent atoms with U_{iso} (H) = 1.2 or 1.5 U_{eq} (C).

Figures

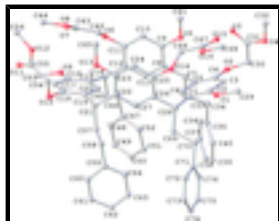


Fig. 1. The molecular structure of the title compound with atomic numbering; the H atoms have been omitted for clarity.

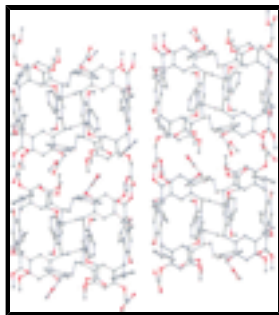


Fig. 2. The packing of the title compound in [100] plane. All hydrogen atoms have been omitted for clarity.

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Crystal data

$C_{76}H_{80}O_{16}$

$M_r = 1249.40$

Monoclinic, $P2_1$

Hall symbol: P 2yb

$a = 14.1361$ (7) Å

$b = 32.2264$ (17) Å

$c = 28.9417$ (16) Å

$\beta = 90.572$ (1)°

$V = 13183.9$ (12) Å³

$Z = 8$

$F(000) = 5312$

PHTMTMES

$D_x = 1.259$ Mg m⁻³

Melting point: 387 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 126694 reflections

$\theta = 1.6$ – 28.3 °

$\mu = 0.09$ mm⁻¹

$T = 173$ K

Block, colourless

$0.41 \times 0.33 \times 0.29$ mm

Data collection

Bruker Kappa DUO APEXII
diffractometer

Radiation source: fine-focus sealed tube
graphite

0.5° φ scans and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2006)

$T_{\min} = 0.965$, $T_{\max} = 0.975$

126671 measured reflections

33391 independent reflections

23289 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.072$

$\theta_{\text{max}} = 28.3^\circ$, $\theta_{\text{min}} = 1.6^\circ$

$h = -18 \rightarrow 18$

$k = -42 \rightarrow 42$

$l = -38 \rightarrow 38$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.056$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.162$	H-atom parameters constrained
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0912P)^2 + 0.241P]$
33391 reflections	where $P = (F_o^2 + 2F_c^2)/3$
3345 parameters	$(\Delta/\sigma)_{\max} = 0.001$
1 restraint	$\Delta\rho_{\max} = 0.44 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$

Special details

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

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

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1A	0.5977 (2)	0.06377 (9)	0.62469 (8)	0.0406 (7)
O2A	0.73848 (19)	0.19974 (8)	0.63413 (8)	0.0345 (6)
O3A	0.8421 (3)	0.15922 (14)	0.70321 (12)	0.0741 (11)
O4A	0.9771 (2)	0.17877 (12)	0.66923 (14)	0.0676 (10)
O5A	0.90039 (17)	0.18472 (9)	0.52995 (8)	0.0353 (6)
O6A	0.91179 (17)	0.19634 (8)	0.36350 (8)	0.0311 (5)
O7A	0.9798 (2)	0.13462 (11)	0.27089 (11)	0.0570 (8)
O8A	1.0272 (2)	0.19763 (9)	0.29379 (9)	0.0448 (7)
O9A	0.7815 (2)	0.20481 (9)	0.26602 (8)	0.0383 (6)
O10A	0.6606 (2)	0.06387 (9)	0.25759 (8)	0.0410 (7)
O11A	0.8362 (3)	0.03043 (16)	0.23211 (16)	0.0933 (15)
O12A	0.8293 (2)	0.07451 (13)	0.17483 (12)	0.0655 (10)
O13A	0.79804 (19)	0.04378 (9)	0.36270 (9)	0.0410 (6)
O14A	0.77605 (17)	0.04228 (8)	0.53017 (8)	0.0305 (5)
O15A	0.9510 (3)	0.08568 (16)	0.60233 (14)	0.0932 (16)
O16A	0.8347 (2)	0.04065 (9)	0.61531 (9)	0.0447 (7)
C1A	0.6302 (2)	0.10053 (10)	0.55664 (11)	0.0249 (7)
C2A	0.6351 (3)	0.09882 (11)	0.60507 (11)	0.0291 (8)

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C3A	0.6740 (3)	0.13123 (12)	0.62974 (11)	0.0319 (8)
H3A	0.6800	0.1293	0.6624	0.038*
C4A	0.7045 (3)	0.16686 (11)	0.60716 (11)	0.0281 (7)
C5A	0.6969 (2)	0.17097 (11)	0.55929 (11)	0.0244 (7)
C6A	0.6609 (2)	0.13684 (10)	0.53538 (10)	0.0241 (7)
H6A	0.6570	0.1384	0.5026	0.029*
C7A	0.7166 (2)	0.21170 (10)	0.53441 (10)	0.0235 (7)
H7A	0.7597	0.2288	0.5544	0.028*
C8A	0.7647 (2)	0.20475 (10)	0.48799 (11)	0.0240 (7)
C9A	0.8593 (2)	0.19183 (11)	0.48741 (11)	0.0250 (7)
C10A	0.9078 (2)	0.18738 (12)	0.44612 (12)	0.0289 (7)
H10A	0.9719	0.1785	0.4463	0.035*
C11A	0.8616 (2)	0.19601 (10)	0.40468 (11)	0.0246 (7)
C12A	0.7668 (2)	0.20724 (10)	0.40281 (11)	0.0248 (7)
C13A	0.7203 (2)	0.21126 (10)	0.44541 (10)	0.0243 (7)
H13A	0.6554	0.2188	0.4451	0.029*
C14A	0.7196 (2)	0.21474 (11)	0.35646 (11)	0.0261 (7)
H14A	0.7629	0.2329	0.3382	0.031*
C15A	0.7084 (2)	0.17450 (11)	0.33004 (10)	0.0251 (7)
C16A	0.7378 (2)	0.17095 (12)	0.28416 (11)	0.0282 (7)
C17A	0.7240 (3)	0.13437 (12)	0.25938 (11)	0.0308 (8)
H17A	0.7439	0.1325	0.2282	0.037*
C18A	0.6811 (3)	0.10060 (12)	0.28029 (11)	0.0311 (8)
C19A	0.6537 (2)	0.10221 (11)	0.32679 (11)	0.0278 (7)
C20A	0.6681 (2)	0.13929 (11)	0.34998 (11)	0.0268 (7)
H20A	0.6494	0.1409	0.3814	0.032*
C21A	0.6119 (3)	0.06472 (12)	0.35088 (11)	0.0295 (8)
H21A	0.6293	0.0396	0.3325	0.035*
C22A	0.6556 (3)	0.05972 (10)	0.39928 (11)	0.0271 (7)
C23A	0.7510 (3)	0.04899 (11)	0.40365 (12)	0.0305 (7)
C24A	0.7927 (2)	0.04358 (11)	0.44714 (12)	0.0296 (7)
H24A	0.8578	0.0367	0.4498	0.035*
C25A	0.7386 (2)	0.04828 (11)	0.48638 (11)	0.0261 (7)
C26A	0.6427 (2)	0.05874 (10)	0.48386 (11)	0.0242 (7)
C27A	0.6043 (2)	0.06467 (10)	0.43976 (11)	0.0250 (7)
H27A	0.5397	0.0725	0.4372	0.030*
C28A	0.5875 (2)	0.06508 (11)	0.52819 (11)	0.0251 (7)
H28A	0.5938	0.0391	0.5469	0.030*
C29A	0.5862 (5)	0.06332 (18)	0.67372 (14)	0.0703 (17)
H29A	0.6481	0.0662	0.6889	0.106*
H29B	0.5572	0.0370	0.6830	0.106*
H29C	0.5454	0.0864	0.6829	0.106*
C30A	0.8390 (3)	0.20284 (14)	0.63534 (13)	0.0378 (9)
H30A	0.8572	0.2323	0.6396	0.045*
H30B	0.8644	0.1935	0.6053	0.045*
C31A	0.8827 (3)	0.17742 (15)	0.67339 (15)	0.0477 (11)
C32A	1.0308 (5)	0.1546 (2)	0.7027 (3)	0.101 (2)
H32A	1.0231	0.1666	0.7336	0.152*
H32B	1.0979	0.1550	0.6945	0.152*

H32C	1.0078	0.1259	0.7027	0.152*
C33A	0.6202 (2)	0.23448 (11)	0.53008 (12)	0.0277 (7)
H33A	0.5799	0.2190	0.5078	0.033*
H33B	0.5887	0.2334	0.5605	0.033*
C34A	0.6245 (3)	0.27998 (11)	0.51453 (12)	0.0305 (7)
H34A	0.6579	0.2966	0.5383	0.037*
H34B	0.6605	0.2820	0.4855	0.037*
C35A	0.5263 (2)	0.29722 (11)	0.50698 (12)	0.0288 (7)
C36A	0.4719 (3)	0.31067 (13)	0.54413 (13)	0.0377 (9)
H36A	0.4983	0.3102	0.5745	0.045*
C37A	0.3806 (3)	0.32462 (14)	0.53750 (15)	0.0453 (10)
H37A	0.3444	0.3333	0.5632	0.054*
C38A	0.3416 (3)	0.32607 (14)	0.49362 (16)	0.0447 (10)
H38A	0.2790	0.3360	0.4890	0.054*
C39A	0.3938 (3)	0.31306 (15)	0.45668 (15)	0.0445 (10)
H39A	0.3669	0.3138	0.4265	0.053*
C40A	0.4859 (3)	0.29885 (14)	0.46317 (13)	0.0399 (9)
H40A	0.5215	0.2901	0.4373	0.048*
C41A	0.9945 (3)	0.16995 (15)	0.53127 (14)	0.0433 (10)
H41A	0.9982	0.1437	0.5143	0.065*
H41B	1.0141	0.1655	0.5634	0.065*
H41C	1.0362	0.1904	0.5169	0.065*
C42A	0.9395 (3)	0.15703 (12)	0.34657 (12)	0.0333 (8)
H42A	0.8836	0.1386	0.3443	0.040*
H42B	0.9857	0.1442	0.3682	0.040*
C43A	0.9834 (3)	0.16199 (13)	0.29944 (13)	0.0379 (9)
C44A	1.0727 (4)	0.20459 (17)	0.25007 (16)	0.0601 (13)
H44A	1.1317	0.1887	0.2490	0.090*
H44B	1.0867	0.2342	0.2466	0.090*
H44C	1.0306	0.1956	0.2249	0.090*
C45A	0.6238 (3)	0.23760 (11)	0.35982 (11)	0.0290 (7)
H45A	0.5770	0.2191	0.3745	0.035*
H45B	0.6315	0.2624	0.3796	0.035*
C46A	0.5866 (3)	0.25087 (16)	0.31208 (13)	0.0473 (11)
H46A	0.6371	0.2659	0.2956	0.057*
H46B	0.5702	0.2258	0.2939	0.057*
C47A	0.5011 (3)	0.27824 (15)	0.31537 (12)	0.0425 (10)
C48A	0.4112 (3)	0.26474 (17)	0.30256 (13)	0.0494 (11)
H48A	0.4024	0.2370	0.2924	0.059*
C49A	0.3340 (3)	0.2913 (2)	0.30441 (15)	0.0573 (14)
H49A	0.2733	0.2817	0.2950	0.069*
C50A	0.3447 (4)	0.3311 (2)	0.31966 (18)	0.0648 (15)
H50A	0.2914	0.3490	0.3212	0.078*
C51A	0.4325 (4)	0.34521 (18)	0.33273 (19)	0.0665 (14)
H51A	0.4404	0.3729	0.3433	0.080*
C52A	0.5091 (3)	0.31913 (17)	0.33049 (16)	0.0536 (12)
H52A	0.5695	0.3293	0.3396	0.064*
C53A	0.8011 (4)	0.20537 (17)	0.21830 (13)	0.0577 (13)
H53A	0.8451	0.1828	0.2110	0.087*

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H53B	0.8298	0.2320	0.2101	0.087*
H53C	0.7422	0.2016	0.2007	0.087*
C54A	0.6866 (3)	0.05979 (14)	0.21032 (13)	0.0407 (9)
H54A	0.6692	0.0854	0.1933	0.049*
H54B	0.6519	0.0363	0.1961	0.049*
C55A	0.7913 (3)	0.05247 (14)	0.20686 (15)	0.0471 (11)
C56A	0.9316 (4)	0.0719 (2)	0.1711 (2)	0.0755 (16)
H56A	0.9596	0.0677	0.2019	0.113*
H56B	0.9560	0.0976	0.1577	0.113*
H56C	0.9482	0.0484	0.1512	0.113*
C57A	0.5038 (3)	0.06717 (13)	0.35165 (11)	0.0325 (8)
H57A	0.4849	0.0932	0.3672	0.039*
H57B	0.4792	0.0437	0.3701	0.039*
C58A	0.4580 (3)	0.06585 (15)	0.30347 (12)	0.0419 (10)
H58A	0.4818	0.0894	0.2850	0.050*
H58B	0.4767	0.0399	0.2878	0.050*
C59A	0.3524 (3)	0.06807 (14)	0.30531 (12)	0.0379 (9)
C60A	0.3049 (3)	0.10405 (16)	0.29462 (14)	0.0479 (11)
H60A	0.3398	0.1275	0.2844	0.057*
C61A	0.2061 (3)	0.1071 (2)	0.29837 (17)	0.0613 (13)
H61A	0.1749	0.1325	0.2915	0.074*
C62A	0.1555 (4)	0.0736 (2)	0.31188 (16)	0.0644 (15)
H62A	0.0886	0.0754	0.3141	0.077*
C63A	0.2002 (4)	0.0374 (2)	0.32229 (17)	0.0691 (17)
H63A	0.1641	0.0140	0.3313	0.083*
C64A	0.2986 (4)	0.03417 (16)	0.31990 (15)	0.0517 (11)
H64A	0.3291	0.0089	0.3282	0.062*
C65A	0.8986 (3)	0.04058 (14)	0.36390 (15)	0.0449 (10)
H65A	0.9248	0.0624	0.3839	0.067*
H65B	0.9233	0.0438	0.3326	0.067*
H65C	0.9169	0.0133	0.3761	0.067*
C66A	0.8643 (3)	0.06057 (17)	0.53789 (14)	0.0505 (11)
H66A	0.8646	0.0887	0.5240	0.061*
H66B	0.9135	0.0439	0.5224	0.061*
C67A	0.8881 (3)	0.06384 (16)	0.58885 (15)	0.0502 (11)
C68A	0.8574 (5)	0.04117 (18)	0.66394 (16)	0.0662 (15)
H68A	0.9216	0.0305	0.6688	0.099*
H68B	0.8123	0.0237	0.6806	0.099*
H68C	0.8538	0.0697	0.6755	0.099*
C69A	0.4809 (2)	0.07354 (11)	0.52119 (12)	0.0296 (7)
H69A	0.4542	0.0822	0.5512	0.035*
H69B	0.4736	0.0972	0.4996	0.035*
C70A	0.4216 (3)	0.03694 (12)	0.50242 (13)	0.0346 (8)
H70A	0.4499	0.0268	0.4734	0.041*
H70B	0.4232	0.0139	0.5251	0.041*
C71A	0.3203 (3)	0.04940 (13)	0.49332 (13)	0.0367 (8)
C72A	0.2949 (3)	0.06849 (15)	0.45133 (15)	0.0474 (10)
H72A	0.3411	0.0719	0.4280	0.057*
C73A	0.2032 (3)	0.08246 (17)	0.44343 (17)	0.0548 (12)

H73A	0.1868	0.0950	0.4147	0.066*
C74A	0.1361 (3)	0.07811 (18)	0.47733 (19)	0.0620 (14)
H74A	0.0736	0.0880	0.4721	0.074*
C75A	0.1591 (3)	0.0596 (2)	0.51867 (17)	0.0628 (15)
H75A	0.1125	0.0563	0.5418	0.075*
C76A	0.2520 (3)	0.04549 (18)	0.52660 (15)	0.0512 (11)
H76A	0.2679	0.0331	0.5554	0.061*
O1B	1.0018 (2)	0.79524 (9)	0.34133 (8)	0.0381 (7)
O2B	0.8747 (2)	0.93555 (9)	0.33391 (8)	0.0411 (7)
O3B	1.0602 (2)	0.95651 (13)	0.32072 (11)	0.0654 (10)
O4B	1.0487 (3)	0.93523 (15)	0.24792 (11)	0.0755 (12)
O5B	1.01302 (19)	0.95766 (10)	0.43576 (8)	0.0399 (7)
O6B	1.00419 (19)	0.96042 (9)	0.60273 (8)	0.0378 (6)
O7B	1.1619 (4)	0.90759 (19)	0.67830 (14)	0.1072 (18)
O8B	1.0632 (3)	0.96019 (13)	0.68735 (11)	0.0770 (12)
O9B	0.8300 (2)	0.93672 (9)	0.70036 (9)	0.0490 (8)
O10B	0.96121 (18)	0.79857 (8)	0.70902 (8)	0.0323 (6)
O11B	1.0645 (3)	0.83863 (15)	0.77772 (13)	0.0826 (13)
O12B	1.2000 (3)	0.81789 (13)	0.74503 (16)	0.0787 (12)
O13B	1.12398 (17)	0.81423 (9)	0.60462 (8)	0.0343 (6)
O14B	1.13407 (18)	0.80255 (8)	0.43820 (8)	0.0334 (6)
O15B	1.1980 (2)	0.86203 (10)	0.34318 (10)	0.0525 (8)
O16B	1.2481 (2)	0.80046 (10)	0.36801 (9)	0.0465 (7)
C1B	0.9267 (2)	0.82519 (11)	0.40523 (11)	0.0250 (7)
C2B	0.9557 (2)	0.82915 (11)	0.35953 (11)	0.0278 (7)
C3B	0.9405 (3)	0.86564 (12)	0.33482 (11)	0.0301 (7)
H3B	0.9603	0.8679	0.3037	0.036*
C4B	0.8957 (3)	0.89890 (11)	0.35642 (11)	0.0289 (7)
C5B	0.8691 (2)	0.89670 (11)	0.40284 (11)	0.0271 (7)
C6B	0.8852 (2)	0.85949 (11)	0.42566 (11)	0.0252 (7)
H6B	0.8668	0.8574	0.4571	0.030*
C7B	0.8277 (2)	0.93422 (11)	0.42711 (11)	0.0259 (7)
H7B	0.8439	0.9591	0.4081	0.031*
C8B	0.8740 (2)	0.94041 (10)	0.47453 (11)	0.0259 (7)
C9B	0.9693 (2)	0.95270 (12)	0.47707 (11)	0.0296 (7)
C10B	1.0125 (3)	0.95889 (12)	0.51966 (12)	0.0336 (8)
H10B	1.0770	0.9671	0.5213	0.040*
C11B	0.9617 (3)	0.95311 (12)	0.56002 (12)	0.0300 (8)
C12B	0.8673 (3)	0.94091 (10)	0.55934 (11)	0.0263 (7)
C13B	0.8265 (2)	0.93461 (10)	0.51559 (11)	0.0258 (7)
H13B	0.7624	0.9258	0.5140	0.031*
C14B	0.8148 (2)	0.93470 (10)	0.60427 (11)	0.0254 (7)
H14B	0.8225	0.9606	0.6230	0.031*
C15B	0.8580 (2)	0.89903 (11)	0.63205 (11)	0.0253 (7)
C16B	0.8635 (3)	0.90096 (11)	0.68041 (11)	0.0314 (8)
C17B	0.9006 (3)	0.86782 (12)	0.70526 (11)	0.0328 (8)
H17B	0.9064	0.8695	0.7379	0.039*
C18B	0.9294 (2)	0.83197 (11)	0.68235 (11)	0.0267 (7)
C19B	0.9210 (2)	0.82820 (11)	0.63443 (10)	0.0242 (7)

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C20B	0.8859 (2)	0.86279 (11)	0.61066 (10)	0.0241 (7)
H20B	0.8809	0.8613	0.5779	0.029*
C21B	0.9388 (2)	0.78750 (10)	0.60906 (10)	0.0235 (7)
H21B	0.9819	0.7703	0.6289	0.028*
C22B	0.9877 (2)	0.79437 (10)	0.56311 (10)	0.0232 (6)
C23B	1.0827 (2)	0.80747 (11)	0.56224 (11)	0.0280 (7)
C24B	1.1303 (2)	0.81150 (11)	0.52095 (12)	0.0289 (7)
H24B	1.1948	0.8197	0.5210	0.035*
C25B	1.0840 (2)	0.80361 (11)	0.47957 (11)	0.0283 (7)
C26B	0.9889 (2)	0.79228 (10)	0.47836 (10)	0.0233 (6)
C27B	0.9430 (2)	0.78827 (10)	0.52042 (11)	0.0238 (7)
H27B	0.8778	0.7810	0.5201	0.029*
C28B	0.9405 (2)	0.78463 (10)	0.43182 (10)	0.0255 (7)
H28B	0.9847	0.7672	0.4133	0.031*
C29B	1.0240 (4)	0.79570 (16)	0.29342 (13)	0.0542 (13)
H29D	0.9665	0.8013	0.2753	0.081*
H29E	1.0500	0.7687	0.2845	0.081*
H29F	1.0708	0.8174	0.2875	0.081*
C30B	0.9087 (3)	0.94058 (14)	0.28801 (13)	0.0406 (9)
H30C	0.8792	0.9654	0.2738	0.049*
H30D	0.8908	0.9161	0.2692	0.049*
C31B	1.0131 (3)	0.94533 (13)	0.28824 (14)	0.0432 (10)
C32B	1.1493 (4)	0.9368 (3)	0.2451 (2)	0.091 (2)
H32D	1.1708	0.9654	0.2500	0.136*
H32E	1.1690	0.9273	0.2145	0.136*
H32F	1.1772	0.9188	0.2689	0.136*
C33B	0.7192 (2)	0.93216 (11)	0.42923 (12)	0.0302 (7)
H33C	0.6958	0.9560	0.4475	0.036*
H33D	0.7005	0.9064	0.4454	0.036*
C34B	0.6721 (3)	0.93296 (13)	0.38107 (13)	0.0377 (9)
H34C	0.6881	0.9593	0.3654	0.045*
H34D	0.6972	0.9098	0.3623	0.045*
C35B	0.5655 (3)	0.92903 (12)	0.38402 (12)	0.0339 (8)
C36B	0.5113 (3)	0.95992 (14)	0.40262 (17)	0.0487 (11)
H36B	0.5413	0.9844	0.4138	0.058*
C37B	0.4139 (3)	0.95647 (15)	0.40565 (17)	0.0505 (11)
H37B	0.3781	0.9783	0.4188	0.061*
C38B	0.3689 (3)	0.92137 (15)	0.38954 (15)	0.0456 (10)
H38B	0.3020	0.9189	0.3910	0.055*
C39B	0.4224 (3)	0.88992 (15)	0.37124 (16)	0.0532 (11)
H39B	0.3924	0.8654	0.3604	0.064*
C40B	0.5193 (3)	0.89365 (14)	0.36853 (15)	0.0457 (10)
H40B	0.5551	0.8716	0.3558	0.055*
C41B	1.1125 (3)	0.96382 (17)	0.43597 (14)	0.0498 (11)
H41D	1.1274	0.9905	0.4506	0.075*
H41E	1.1354	0.9638	0.4041	0.075*
H41F	1.1432	0.9414	0.4533	0.075*
C42B	1.0814 (3)	0.93282 (17)	0.61229 (15)	0.0508 (11)
H42C	1.1374	0.9417	0.5945	0.061*

H42D	1.0642	0.9044	0.6022	0.061*
C43B	1.1059 (4)	0.93229 (19)	0.66253 (17)	0.0587 (13)
C44B	1.0826 (7)	0.9580 (3)	0.73696 (19)	0.122 (3)
H44D	1.0856	0.9289	0.7466	0.182*
H44E	1.0320	0.9721	0.7537	0.182*
H44F	1.1432	0.9716	0.7438	0.182*
C45B	0.7084 (2)	0.92626 (11)	0.59904 (12)	0.0301 (7)
H45C	0.6837	0.9177	0.6295	0.036*
H45D	0.6996	0.9026	0.5776	0.036*
C46B	0.6486 (3)	0.96285 (12)	0.58115 (13)	0.0342 (8)
H46C	0.6496	0.9854	0.6044	0.041*
H46D	0.6767	0.9737	0.5524	0.041*
C47B	0.5467 (3)	0.95015 (13)	0.57156 (13)	0.0357 (8)
C48B	0.4740 (3)	0.96187 (17)	0.60043 (15)	0.0520 (11)
H48B	0.4877	0.9784	0.6269	0.062*
C49B	0.3815 (3)	0.9498 (2)	0.59131 (18)	0.0629 (14)
H49B	0.3328	0.9580	0.6118	0.076*
C50B	0.3594 (4)	0.92652 (18)	0.55356 (19)	0.0589 (13)
H50B	0.2957	0.9187	0.5475	0.071*
C51B	0.4312 (4)	0.91425 (17)	0.52382 (18)	0.0581 (13)
H51B	0.4172	0.8976	0.4975	0.070*
C52B	0.5236 (3)	0.92668 (14)	0.53327 (15)	0.0475 (10)
H52B	0.5722	0.9188	0.5127	0.057*
C53B	0.8138 (6)	0.9361 (2)	0.74848 (17)	0.107 (3)
H53D	0.7837	0.9098	0.7570	0.161*
H53E	0.7722	0.9592	0.7567	0.161*
H53F	0.8742	0.9389	0.7651	0.161*
C54B	1.0612 (3)	0.79463 (14)	0.71023 (13)	0.0409 (9)
H54C	1.0872	0.8039	0.6803	0.049*
H54D	1.0783	0.7651	0.7145	0.049*
C55B	1.1053 (4)	0.82009 (16)	0.74905 (17)	0.0551 (12)
C56B	1.2510 (6)	0.8419 (3)	0.7793 (4)	0.137 (4)
H56D	1.2421	0.8715	0.7731	0.206*
H56E	1.3184	0.8350	0.7780	0.206*
H56F	1.2269	0.8353	0.8101	0.206*
C57B	0.8434 (2)	0.76435 (11)	0.60507 (11)	0.0258 (7)
H57C	0.8126	0.7651	0.6356	0.031*
H57D	0.8022	0.7798	0.5832	0.031*
C58B	0.8481 (2)	0.71897 (11)	0.58905 (12)	0.0286 (7)
H58C	0.8839	0.7174	0.5599	0.034*
H58D	0.8823	0.7023	0.6126	0.034*
C59B	0.7506 (3)	0.70113 (11)	0.58152 (12)	0.0289 (8)
C60B	0.6953 (3)	0.68891 (13)	0.61846 (13)	0.0383 (9)
H60B	0.7206	0.6904	0.6490	0.046*
C61B	0.6039 (3)	0.67455 (14)	0.61158 (15)	0.0445 (10)
H61B	0.5671	0.6663	0.6373	0.053*
C62B	0.5663 (3)	0.67216 (14)	0.56751 (16)	0.0456 (10)
H62B	0.5035	0.6624	0.5629	0.055*
C63B	0.6191 (3)	0.68378 (15)	0.53057 (15)	0.0460 (10)

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H63B	0.5938	0.6817	0.5001	0.055*
C64B	0.7104 (3)	0.69868 (14)	0.53772 (13)	0.0387 (9)
H64B	0.7462	0.7074	0.5119	0.046*
C65B	1.2191 (3)	0.82781 (16)	0.60531 (14)	0.0455 (10)
H65D	1.2583	0.8081	0.5883	0.068*
H65E	1.2418	0.8296	0.6374	0.068*
H65F	1.2233	0.8552	0.5908	0.068*
C66B	1.1609 (3)	0.84164 (12)	0.42021 (13)	0.0347 (8)
H66C	1.2079	0.8548	0.4411	0.042*
H66D	1.1048	0.8600	0.4181	0.042*
C67B	1.2034 (3)	0.83606 (13)	0.37231 (14)	0.0376 (9)
C68B	1.2921 (4)	0.79220 (17)	0.32324 (16)	0.0632 (14)
H68D	1.2434	0.7837	0.3008	0.095*
H68E	1.3390	0.7700	0.3267	0.095*
H68F	1.3235	0.8174	0.3122	0.095*
C69B	0.8477 (3)	0.76057 (11)	0.43491 (11)	0.0290 (7)
H69C	0.7991	0.7784	0.4492	0.035*
H69D	0.8571	0.7360	0.4550	0.035*
C70B	0.8125 (3)	0.74636 (15)	0.38724 (13)	0.0461 (11)
H70C	0.7954	0.7711	0.3686	0.055*
H70D	0.8644	0.7318	0.3713	0.055*
C71B	0.7280 (3)	0.71796 (15)	0.38978 (12)	0.0443 (10)
C72B	0.7407 (4)	0.67666 (16)	0.40247 (16)	0.0561 (13)
H72B	0.8022	0.6669	0.4102	0.067*
C73B	0.6645 (4)	0.6497 (2)	0.40400 (19)	0.0738 (17)
H73B	0.6739	0.6216	0.4129	0.089*
C74B	0.5767 (4)	0.6633 (2)	0.39283 (18)	0.0747 (18)
H74B	0.5249	0.6446	0.3937	0.090*
C75B	0.5619 (4)	0.7033 (2)	0.38035 (16)	0.0666 (16)
H75B	0.5000	0.7125	0.3723	0.080*
C76B	0.6388 (4)	0.73129 (18)	0.37936 (15)	0.0568 (13)
H76B	0.6283	0.7595	0.3714	0.068*
O1C	0.6334 (2)	0.42533 (8)	0.78498 (8)	0.0386 (6)
O2C	0.54013 (19)	0.28157 (8)	0.78784 (8)	0.0340 (6)
O3C	0.4306 (3)	0.31475 (14)	0.71475 (13)	0.0790 (13)
O4C	0.3017 (3)	0.30626 (12)	0.75901 (13)	0.0643 (10)
O5C	0.37492 (17)	0.30624 (9)	0.88976 (8)	0.0348 (6)
O6C	0.36534 (17)	0.30811 (8)	1.05676 (8)	0.0305 (5)
O7C	0.2863 (3)	0.38220 (12)	1.13619 (12)	0.0658 (10)
O8C	0.2486 (3)	0.31538 (11)	1.12528 (11)	0.0648 (10)
O9C	0.5012 (2)	0.29777 (9)	1.15672 (8)	0.0399 (7)
C54C	0.4775 (4)	0.45404 (17)	1.18003 (18)	0.0640 (14)
H54E	0.4546	0.4828	1.1750	0.077*
H54F	0.4239	0.4353	1.1727	0.077*
O11C	0.4449 (5)	0.4576 (3)	1.2572 (2)	0.167 (3)
O12C	0.5856 (4)	0.43490 (14)	1.23654 (14)	0.0871 (13)
O13C	0.43808 (19)	0.45772 (9)	1.04240 (9)	0.0391 (6)
O14C	0.46610 (18)	0.45251 (9)	0.87540 (9)	0.0355 (6)
O15C	0.2899 (3)	0.40794 (18)	0.80443 (14)	0.1036 (18)

O16C	0.3992 (2)	0.45611 (11)	0.79010 (10)	0.0521 (8)
C1C	0.6202 (2)	0.39033 (11)	0.85618 (11)	0.0265 (7)
C2C	0.6113 (3)	0.38904 (11)	0.80786 (11)	0.0287 (7)
C3C	0.5836 (3)	0.35322 (12)	0.78595 (12)	0.0316 (8)
H3C	0.5769	0.3527	0.7533	0.038*
C4C	0.5652 (2)	0.31767 (11)	0.81153 (11)	0.0278 (7)
C5C	0.5737 (2)	0.31754 (10)	0.85965 (11)	0.0241 (7)
C6C	0.6012 (2)	0.35415 (11)	0.88070 (11)	0.0256 (7)
H6C	0.6073	0.3547	0.9134	0.031*
C7C	0.5593 (2)	0.27790 (11)	0.88806 (10)	0.0248 (7)
H7C	0.5171	0.2591	0.8697	0.030*
C8C	0.5098 (2)	0.28729 (10)	0.93314 (11)	0.0249 (7)
C9C	0.4158 (2)	0.30155 (11)	0.93275 (11)	0.0266 (7)
C10C	0.3688 (2)	0.30952 (11)	0.97340 (12)	0.0282 (7)
H10C	0.3052	0.3191	0.9724	0.034*
C11C	0.4141 (2)	0.30364 (11)	1.01567 (11)	0.0263 (7)
C12C	0.5077 (2)	0.29059 (10)	1.01802 (11)	0.0236 (6)
C13C	0.5531 (2)	0.28308 (10)	0.97614 (11)	0.0237 (6)
H13C	0.6174	0.2746	0.9772	0.028*
C14C	0.5554 (2)	0.28570 (10)	1.06485 (11)	0.0254 (7)
H14C	0.5138	0.2675	1.0839	0.031*
C15C	0.5604 (2)	0.32745 (11)	1.08878 (11)	0.0269 (7)
C16C	0.5293 (3)	0.33302 (11)	1.13396 (11)	0.0293 (7)
C17C	0.5266 (3)	0.37189 (12)	1.15397 (12)	0.0351 (8)
H17C	0.5057	0.3751	1.1849	0.042*
C18C	0.5547 (3)	0.40638 (12)	1.12853 (12)	0.0332 (8)
C19C	0.5906 (3)	0.40237 (11)	1.08402 (11)	0.0286 (7)
C20C	0.5910 (2)	0.36275 (11)	1.06521 (11)	0.0266 (7)
H20C	0.6134	0.3594	1.0346	0.032*
C21C	0.6269 (3)	0.43926 (11)	1.05680 (11)	0.0290 (7)
H21C	0.6070	0.4649	1.0736	0.035*
C22C	0.5836 (2)	0.44144 (10)	1.00860 (11)	0.0276 (7)
C23C	0.4878 (3)	0.45137 (11)	1.00251 (12)	0.0301 (7)
C24C	0.4474 (3)	0.45469 (12)	0.95842 (12)	0.0321 (8)
H24C	0.3824	0.4616	0.9548	0.039*
C25C	0.5032 (3)	0.44785 (11)	0.92012 (11)	0.0296 (7)
C26C	0.5989 (2)	0.43753 (10)	0.92381 (11)	0.0252 (7)
C27C	0.6360 (3)	0.43464 (10)	0.96877 (11)	0.0272 (7)
H27C	0.7009	0.4276	0.9723	0.033*
C28C	0.6560 (2)	0.42890 (11)	0.88075 (11)	0.0273 (7)
H28C	0.6475	0.4530	0.8593	0.033*
C29C	0.6183 (4)	0.42511 (17)	0.73575 (14)	0.0584 (13)
H29G	0.6635	0.4061	0.7213	0.088*
H29H	0.6274	0.4532	0.7236	0.088*
H29I	0.5536	0.4158	0.7288	0.088*
C30C	0.4399 (3)	0.27555 (13)	0.78595 (13)	0.0378 (9)
H30E	0.4123	0.2831	0.8161	0.045*
H30F	0.4261	0.2459	0.7802	0.045*
C31C	0.3940 (4)	0.30163 (14)	0.74807 (16)	0.0489 (11)

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C32C	0.2466 (5)	0.3300 (2)	0.7255 (3)	0.103 (3)
H32G	0.2721	0.3582	0.7234	0.154*
H32H	0.1805	0.3312	0.7353	0.154*
H32I	0.2500	0.3165	0.6952	0.154*
C33C	0.6552 (2)	0.25617 (11)	0.89332 (12)	0.0286 (7)
H33E	0.6954	0.2728	0.9146	0.034*
H33F	0.6864	0.2559	0.8628	0.034*
C34C	0.6513 (3)	0.21142 (11)	0.91156 (12)	0.0312 (8)
H34E	0.6181	0.2111	0.9415	0.037*
H34F	0.6145	0.1941	0.8896	0.037*
C35C	0.7494 (3)	0.19285 (12)	0.91794 (13)	0.0314 (8)
C36C	0.7943 (4)	0.17242 (16)	0.88213 (15)	0.0532 (12)
H36C	0.7625	0.1689	0.8533	0.064*
C37C	0.8855 (4)	0.15704 (17)	0.88807 (17)	0.0632 (14)
H37C	0.9155	0.1433	0.8632	0.076*
C38C	0.9323 (3)	0.16145 (15)	0.92905 (18)	0.0532 (12)
H38C	0.9946	0.1509	0.9328	0.064*
C39C	0.8886 (3)	0.18131 (15)	0.96496 (17)	0.0512 (11)
H39C	0.9203	0.1842	0.9939	0.061*
C40C	0.7975 (3)	0.19727 (14)	0.95899 (14)	0.0434 (10)
H40C	0.7684	0.2115	0.9838	0.052*
C41C	0.2804 (3)	0.32222 (15)	0.88786 (15)	0.0456 (10)
H41G	0.2375	0.3027	0.9030	0.068*
H41H	0.2608	0.3258	0.8555	0.068*
H41I	0.2781	0.3491	0.9037	0.068*
C42C	0.3361 (3)	0.34942 (12)	1.06685 (13)	0.0355 (8)
H42E	0.2914	0.3591	1.0426	0.043*
H42F	0.3918	0.3681	1.0669	0.043*
C43C	0.2889 (3)	0.35114 (14)	1.11333 (14)	0.0444 (10)
C44C	0.1966 (5)	0.3146 (2)	1.1685 (2)	0.089 (2)
H44G	0.2370	0.3252	1.1935	0.134*
H44H	0.1775	0.2861	1.1754	0.134*
H44I	0.1401	0.3321	1.1655	0.134*
C45C	0.6529 (3)	0.26473 (12)	1.06296 (12)	0.0321 (8)
H45E	0.6479	0.2392	1.0440	0.039*
H45F	0.6980	0.2837	1.0477	0.039*
C46C	0.6913 (3)	0.25344 (15)	1.11070 (13)	0.0456 (10)
H46E	0.7061	0.2792	1.1279	0.055*
H46F	0.6419	0.2383	1.1279	0.055*
C47C	0.7798 (3)	0.22670 (15)	1.10839 (12)	0.0452 (11)
C48C	0.7739 (4)	0.18567 (16)	1.09488 (16)	0.0540 (12)
H48C	0.7140	0.1742	1.0869	0.065*
C49C	0.8535 (4)	0.16114 (19)	1.09284 (19)	0.0649 (14)
H49C	0.8488	0.1333	1.0824	0.078*
C50C	0.9399 (4)	0.1771 (2)	1.10603 (18)	0.0634 (14)
H50C	0.9945	0.1600	1.1058	0.076*
C51C	0.9474 (3)	0.21738 (18)	1.11938 (14)	0.0526 (12)
H51C	1.0071	0.2285	1.1282	0.063*
C52C	0.8672 (3)	0.24233 (17)	1.12010 (14)	0.0515 (11)

H52C	0.8730	0.2706	1.1288	0.062*
C53C	0.4736 (5)	0.30092 (18)	1.20303 (13)	0.0723 (19)
H53G	0.5256	0.3127	1.2214	0.108*
H53H	0.4578	0.2733	1.2148	0.108*
H53I	0.4180	0.3190	1.2051	0.108*
O10C	0.5506 (2)	0.44617 (9)	1.14663 (9)	0.0484 (7)
C55C	0.4986 (5)	0.4497 (2)	1.2281 (2)	0.0775 (18)
C56C	0.6140 (7)	0.4280 (3)	1.2873 (2)	0.127 (3)
H56G	0.6258	0.4549	1.3021	0.190*
H56H	0.6715	0.4111	1.2889	0.190*
H56I	0.5627	0.4137	1.3034	0.190*
C57C	0.7351 (3)	0.43904 (12)	1.05619 (12)	0.0320 (8)
H57E	0.7568	0.4133	1.0410	0.038*
H57F	0.7572	0.4628	1.0375	0.038*
C58C	0.7801 (3)	0.44175 (13)	1.10428 (13)	0.0412 (9)
H58E	0.7643	0.4690	1.1180	0.049*
H58F	0.7521	0.4200	1.1241	0.049*
C59C	0.8861 (3)	0.43667 (13)	1.10470 (15)	0.0457 (11)
C60C	0.9422 (3)	0.45302 (15)	1.07105 (19)	0.0584 (13)
H60C	0.9136	0.4687	1.0468	0.070*
C61C	1.0395 (4)	0.44750 (17)	1.0711 (2)	0.0699 (16)
H61C	1.0767	0.4594	1.0473	0.084*
C62C	1.0818 (4)	0.42485 (19)	1.1057 (3)	0.081 (2)
H62C	1.1482	0.4202	1.1057	0.097*
C63C	1.0268 (5)	0.4090 (2)	1.1403 (2)	0.081 (2)
H63C	1.0559	0.3944	1.1651	0.097*
C64C	0.9305 (4)	0.41407 (17)	1.13970 (17)	0.0653 (15)
H64C	0.8936	0.4020	1.1634	0.078*
C65C	0.3383 (3)	0.46367 (17)	1.03865 (16)	0.0518 (11)
H65G	0.3252	0.4907	1.0245	0.078*
H65H	0.3103	0.4627	1.0695	0.078*
H65I	0.3107	0.4417	1.0194	0.078*
C66C	0.3882 (4)	0.4269 (2)	0.86587 (16)	0.080 (2)
H66E	0.3356	0.4348	0.8864	0.096*
H66F	0.4056	0.3978	0.8731	0.096*
C67C	0.3544 (4)	0.42902 (19)	0.81719 (16)	0.0621 (14)
C68C	0.3666 (4)	0.4575 (2)	0.74228 (15)	0.0662 (15)
H68G	0.3594	0.4291	0.7305	0.099*
H68H	0.4129	0.4724	0.7236	0.099*
H68I	0.3055	0.4718	0.7406	0.099*
C69C	0.7634 (2)	0.42304 (11)	0.88933 (12)	0.0311 (8)
H69E	0.7720	0.4018	0.9137	0.037*
H69F	0.7915	0.4118	0.8607	0.037*
C70C	0.8198 (3)	0.46189 (12)	0.90363 (14)	0.0356 (8)
H70E	0.8090	0.4844	0.8809	0.043*
H70F	0.7987	0.4717	0.9342	0.043*
C71C	0.9229 (3)	0.45106 (13)	0.90571 (16)	0.0449 (10)
C72C	0.9594 (3)	0.42801 (17)	0.9421 (2)	0.0673 (15)
H72C	0.9192	0.4208	0.9669	0.081*

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C73C	1.0525 (5)	0.4152 (2)	0.9431 (3)	0.110 (3)
H73C	1.0771	0.4000	0.9687	0.132*
C74C	1.1092 (4)	0.4251 (2)	0.9060 (5)	0.132 (4)
H74C	1.1727	0.4156	0.9056	0.159*
C75C	1.0752 (5)	0.4489 (3)	0.8691 (3)	0.109 (3)
H75C	1.1156	0.4562	0.8444	0.131*
C76C	0.9810 (4)	0.46159 (19)	0.8690 (2)	0.0682 (15)
H76C	0.9565	0.4774	0.8440	0.082*
O1D	0.8576 (2)	0.57303 (8)	0.85863 (8)	0.0347 (6)
O2D	0.76530 (17)	0.71659 (8)	0.86430 (8)	0.0314 (5)
O3D	0.6548 (3)	0.68559 (14)	0.78997 (11)	0.0698 (11)
O4D	0.5299 (2)	0.68868 (11)	0.83635 (12)	0.0603 (9)
O5D	0.60316 (16)	0.69184 (8)	0.96648 (8)	0.0309 (5)
O6D	0.59365 (17)	0.69021 (7)	1.13331 (8)	0.0283 (5)
O7D	0.4997 (2)	0.61489 (10)	1.20839 (11)	0.0564 (8)
O8D	0.4720 (2)	0.68293 (9)	1.20022 (10)	0.0488 (7)
O9D	0.7279 (2)	0.69822 (10)	1.23279 (9)	0.0460 (8)
O10D	0.7668 (2)	0.54882 (10)	1.21833 (9)	0.0466 (7)
O11D	0.6741 (4)	0.5312 (2)	1.33062 (14)	0.130 (2)
O12D	0.8111 (3)	0.55522 (15)	1.30678 (11)	0.0768 (12)
O13D	0.65440 (18)	0.54636 (9)	1.11335 (8)	0.0343 (6)
O14D	0.69516 (16)	0.54863 (8)	0.94702 (7)	0.0293 (5)
O15D	0.4968 (3)	0.56939 (16)	0.87660 (11)	0.0835 (14)
O16D	0.62933 (19)	0.53456 (9)	0.86243 (8)	0.0390 (6)
C1D	0.8491 (2)	0.60721 (11)	0.93081 (10)	0.0242 (7)
C2D	0.8376 (2)	0.60882 (11)	0.88217 (11)	0.0256 (7)
C3D	0.8090 (2)	0.64512 (11)	0.86101 (11)	0.0282 (7)
H3D	0.8011	0.6461	0.8284	0.034*
C4D	0.7917 (2)	0.68037 (11)	0.88744 (11)	0.0258 (7)
C5D	0.8012 (2)	0.68024 (11)	0.93557 (11)	0.0244 (7)
C6D	0.8304 (2)	0.64293 (10)	0.95560 (10)	0.0238 (7)
H6D	0.8379	0.6420	0.9882	0.029*
C7D	0.7879 (2)	0.71927 (10)	0.96432 (10)	0.0235 (6)
H7D	0.7455	0.7383	0.9463	0.028*
C8D	0.7386 (2)	0.70960 (10)	1.00988 (10)	0.0226 (6)
C9D	0.6447 (2)	0.69641 (11)	1.00945 (11)	0.0256 (7)
C10D	0.5967 (2)	0.68893 (11)	1.05020 (11)	0.0266 (7)
H10D	0.5326	0.6800	1.0494	0.032*
C11D	0.6433 (2)	0.69465 (10)	1.09212 (11)	0.0249 (7)
C12D	0.7368 (2)	0.70689 (10)	1.09453 (11)	0.0246 (7)
C13D	0.7833 (2)	0.71382 (10)	1.05297 (11)	0.0242 (7)
H13D	0.8480	0.7217	1.0540	0.029*
C14D	0.7859 (2)	0.71099 (11)	1.14178 (11)	0.0269 (7)
H14D	0.7451	0.7293	1.1611	0.032*
C15D	0.7879 (2)	0.66872 (12)	1.16476 (10)	0.0271 (7)
C16D	0.7543 (3)	0.66291 (13)	1.20978 (11)	0.0330 (8)
C17D	0.7475 (3)	0.62339 (13)	1.22849 (12)	0.0377 (9)
H17D	0.7246	0.6197	1.2590	0.045*
C18D	0.7746 (3)	0.58907 (13)	1.20216 (12)	0.0353 (8)

C19D	0.8114 (2)	0.59367 (11)	1.15822 (11)	0.0275 (7)
C20D	0.8168 (2)	0.63369 (11)	1.14096 (10)	0.0261 (7)
H20D	0.8418	0.6374	1.1109	0.031*
C21D	0.8465 (3)	0.55645 (11)	1.13036 (11)	0.0291 (7)
H21D	0.8230	0.5309	1.1461	0.035*
C22D	0.8051 (2)	0.55628 (10)	1.08138 (10)	0.0262 (7)
C23D	0.7085 (2)	0.55013 (11)	1.07421 (11)	0.0273 (7)
C24D	0.6699 (2)	0.54738 (11)	1.02982 (11)	0.0268 (7)
H24D	0.6041	0.5427	1.0256	0.032*
C25D	0.7285 (2)	0.55150 (11)	0.99182 (11)	0.0240 (7)
C26D	0.8247 (2)	0.55976 (11)	0.99720 (11)	0.0241 (7)
C27D	0.8603 (2)	0.56165 (10)	1.04224 (11)	0.0252 (7)
H27D	0.9259	0.5669	1.0465	0.030*
C28D	0.8848 (2)	0.56808 (11)	0.95450 (11)	0.0246 (7)
H28D	0.8763	0.5443	0.9326	0.030*
C29D	0.8370 (3)	0.57293 (14)	0.81022 (12)	0.0431 (10)
H29J	0.7715	0.5819	0.8050	0.065*
H29K	0.8453	0.5448	0.7980	0.065*
H29L	0.8799	0.5920	0.7945	0.065*
C30D	0.6645 (3)	0.72198 (13)	0.86260 (13)	0.0355 (8)
H30G	0.6498	0.7516	0.8572	0.043*
H30H	0.6375	0.7140	0.8927	0.043*
C31D	0.6195 (3)	0.69637 (13)	0.82514 (15)	0.0428 (10)
C32D	0.4737 (5)	0.6647 (2)	0.8036 (2)	0.090 (2)
H32J	0.4677	0.6802	0.7745	0.136*
H32K	0.4107	0.6598	0.8163	0.136*
H32L	0.5049	0.6381	0.7978	0.136*
C33D	0.8841 (2)	0.74125 (11)	0.97000 (11)	0.0270 (7)
H33G	0.9240	0.7247	0.9914	0.032*
H33H	0.9158	0.7415	0.9397	0.032*
C34D	0.8800 (2)	0.78596 (12)	0.98813 (12)	0.0304 (7)
H34G	0.8448	0.8035	0.9658	0.036*
H34H	0.8457	0.7865	1.0178	0.036*
C35D	0.9782 (3)	0.80352 (11)	0.99530 (13)	0.0301 (8)
C36D	1.0259 (3)	0.82269 (13)	0.95902 (14)	0.0419 (9)
H36D	0.9954	0.8263	0.9299	0.050*
C37D	1.1190 (3)	0.83655 (15)	0.96579 (16)	0.0513 (11)
H37D	1.1519	0.8489	0.9408	0.062*
C38D	1.1633 (3)	0.83252 (14)	1.00781 (17)	0.0482 (11)
H38D	1.2261	0.8423	1.0120	0.058*
C39D	1.1164 (3)	0.81424 (15)	1.04392 (16)	0.0477 (10)
H39D	1.1469	0.8115	1.0732	0.057*
C40D	1.0241 (3)	0.79977 (14)	1.03774 (14)	0.0397 (9)
H40D	0.9923	0.7872	1.0629	0.048*
C41D	0.5119 (3)	0.67344 (15)	0.96403 (13)	0.0423 (10)
H41J	0.5134	0.6464	0.9795	0.063*
H41K	0.4933	0.6697	0.9316	0.063*
H41L	0.4661	0.6915	0.9793	0.063*
C42D	0.5611 (3)	0.64925 (11)	1.14234 (13)	0.0320 (8)

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H42G	0.6157	0.6300	1.1432	0.038*
H42H	0.5182	0.6403	1.1170	0.038*
C43D	0.5093 (3)	0.64697 (13)	1.18770 (13)	0.0371 (9)
C44D	0.4151 (4)	0.68332 (18)	1.24156 (17)	0.0702 (16)
H44J	0.3552	0.6689	1.2355	0.105*
H44K	0.4022	0.7121	1.2505	0.105*
H44L	0.4493	0.6693	1.2666	0.105*
C45D	0.8834 (3)	0.73162 (12)	1.13942 (11)	0.0304 (8)
H45G	0.9279	0.7127	1.1237	0.037*
H45H	0.8785	0.7573	1.1208	0.037*
C46D	0.9228 (3)	0.74229 (16)	1.18744 (13)	0.0471 (11)
H46G	0.8728	0.7561	1.2056	0.057*
H46H	0.9406	0.7164	1.2037	0.057*
C47D	1.0080 (3)	0.77037 (16)	1.18500 (12)	0.0456 (11)
C48D	0.9991 (4)	0.81137 (17)	1.17239 (15)	0.0546 (12)
H48D	0.9384	0.8216	1.1637	0.065*
C49D	1.0755 (4)	0.83820 (19)	1.17188 (18)	0.0640 (14)
H49D	1.0672	0.8665	1.1634	0.077*
C50D	1.1646 (4)	0.8232 (2)	1.18391 (16)	0.0617 (14)
H50D	1.2179	0.8411	1.1833	0.074*
C51D	1.1753 (3)	0.78279 (19)	1.19651 (14)	0.0546 (13)
H51D	1.2360	0.7727	1.2054	0.066*
C52D	1.0980 (3)	0.75608 (17)	1.19643 (13)	0.0500 (11)
H52D	1.1068	0.7277	1.2043	0.060*
C53D	0.6941 (5)	0.69408 (19)	1.27797 (13)	0.0715 (18)
H53J	0.6363	0.6773	1.2776	0.107*
H53K	0.6802	0.7216	1.2906	0.107*
H53L	0.7422	0.6804	1.2973	0.107*
C54D	0.6951 (4)	0.54023 (18)	1.25043 (16)	0.0583 (13)
H54G	0.6703	0.5121	1.2440	0.070*
H54H	0.6427	0.5601	1.2451	0.070*
C55D	0.7230 (4)	0.54227 (17)	1.30033 (16)	0.0599 (13)
C56D	0.8448 (6)	0.5573 (3)	1.3548 (2)	0.110 (3)
H56J	0.8061	0.5771	1.3720	0.165*
H56K	0.9110	0.5664	1.3554	0.165*
H56L	0.8400	0.5298	1.3690	0.165*
C57D	0.9557 (3)	0.55471 (12)	1.13162 (11)	0.0329 (8)
H57G	0.9777	0.5333	1.1096	0.039*
H57H	0.9814	0.5818	1.1216	0.039*
C58D	0.9938 (3)	0.54457 (18)	1.17988 (14)	0.0523 (12)
H58G	0.9627	0.5629	1.2026	0.063*
H58H	0.9767	0.5156	1.1876	0.063*
C59D	1.0996 (3)	0.54957 (14)	1.18446 (13)	0.0436 (10)
C60D	1.1596 (4)	0.52542 (19)	1.1591 (2)	0.0725 (17)
H60D	1.1342	0.5057	1.1381	0.087*
C61D	1.2574 (5)	0.5293 (3)	1.1637 (2)	0.099 (2)
H61D	1.2975	0.5113	1.1469	0.119*
C62D	1.2964 (4)	0.5588 (2)	1.1921 (2)	0.0765 (18)
H62D	1.3630	0.5625	1.1941	0.092*

C63D	1.2372 (5)	0.5823 (2)	1.2172 (2)	0.0758 (18)
H63D	1.2630	0.6023	1.2379	0.091*
C64D	1.1388 (4)	0.57823 (18)	1.21380 (16)	0.0617 (14)
H64D	1.0991	0.5954	1.2319	0.074*
C65D	0.5544 (3)	0.54612 (13)	1.10817 (13)	0.0381 (8)
H65J	0.5347	0.5696	1.0888	0.057*
H65K	0.5251	0.5485	1.1386	0.057*
H65L	0.5344	0.5201	1.0935	0.057*
C66D	0.5971 (3)	0.55178 (15)	0.94016 (13)	0.0438 (10)
H66G	0.5737	0.5771	0.9558	0.053*
H66H	0.5658	0.5275	0.9544	0.053*
C67D	0.5703 (3)	0.55367 (16)	0.88947 (13)	0.0485 (11)
C68D	0.5984 (4)	0.53020 (16)	0.81441 (14)	0.0506 (12)
H68J	0.5426	0.5122	0.8129	0.076*
H68K	0.6495	0.5179	0.7963	0.076*
H68L	0.5825	0.5576	0.8018	0.076*
C69D	0.9912 (2)	0.57360 (11)	0.96396 (12)	0.0302 (7)
H69G	1.0200	0.5850	0.9356	0.036*
H69H	0.9987	0.5948	0.9885	0.036*
C70D	1.0484 (3)	0.53524 (13)	0.97847 (14)	0.0396 (9)
H70G	1.0230	0.5239	1.0076	0.047*
H70H	1.0425	0.5135	0.9544	0.047*
C71D	1.1510 (3)	0.54668 (14)	0.98517 (17)	0.0455 (10)
C72D	1.2143 (4)	0.5444 (2)	0.9493 (2)	0.0774 (19)
H72D	1.1956	0.5325	0.9206	0.093*
C73D	1.3082 (5)	0.5601 (3)	0.9557 (4)	0.114 (3)
H73D	1.3522	0.5596	0.9311	0.137*
C74D	1.3337 (6)	0.5760 (3)	0.9986 (5)	0.129 (4)
H74D	1.3964	0.5860	1.0030	0.155*
C75D	1.2723 (5)	0.5779 (2)	1.0348 (4)	0.104 (3)
H75D	1.2912	0.5887	1.0640	0.125*
C76D	1.1820 (4)	0.56335 (17)	1.0270 (2)	0.0694 (15)
H76D	1.1382	0.5648	1.0517	0.083*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0616 (19)	0.0339 (15)	0.0263 (12)	-0.0052 (13)	0.0100 (12)	0.0060 (11)
O2A	0.0409 (15)	0.0331 (14)	0.0295 (12)	-0.0001 (11)	-0.0042 (11)	-0.0062 (11)
O3A	0.065 (2)	0.097 (3)	0.060 (2)	0.000 (2)	-0.0179 (18)	0.033 (2)
O4A	0.046 (2)	0.067 (2)	0.089 (3)	-0.0014 (17)	-0.0245 (18)	0.008 (2)
O5A	0.0232 (13)	0.0501 (17)	0.0326 (12)	0.0078 (12)	-0.0048 (10)	0.0064 (11)
O6A	0.0315 (13)	0.0301 (13)	0.0320 (12)	0.0043 (10)	0.0110 (10)	0.0004 (10)
O7A	0.070 (2)	0.053 (2)	0.0483 (17)	-0.0019 (17)	0.0149 (15)	-0.0148 (15)
O8A	0.0508 (17)	0.0421 (17)	0.0420 (15)	-0.0003 (14)	0.0229 (13)	-0.0021 (12)
O9A	0.0522 (17)	0.0398 (15)	0.0232 (12)	-0.0069 (13)	0.0107 (11)	0.0041 (11)
O10A	0.0555 (18)	0.0407 (16)	0.0272 (12)	-0.0047 (13)	0.0108 (11)	-0.0080 (11)
O11A	0.066 (3)	0.110 (4)	0.105 (3)	0.031 (2)	0.014 (2)	0.053 (3)

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O12A	0.052 (2)	0.087 (3)	0.0577 (19)	0.0113 (18)	0.0157 (15)	0.0225 (18)
O13A	0.0365 (15)	0.0507 (17)	0.0360 (13)	0.0109 (13)	0.0164 (11)	-0.0010 (12)
O14A	0.0254 (12)	0.0317 (13)	0.0342 (12)	-0.0006 (10)	0.0006 (10)	0.0061 (10)
O15A	0.093 (3)	0.117 (4)	0.068 (2)	-0.058 (3)	-0.039 (2)	0.026 (2)
O16A	0.0553 (18)	0.0403 (17)	0.0386 (14)	-0.0041 (14)	-0.0009 (12)	0.0023 (12)
C1A	0.0263 (17)	0.0243 (17)	0.0242 (15)	0.0037 (13)	0.0028 (12)	0.0003 (12)
C2A	0.036 (2)	0.0258 (18)	0.0258 (16)	0.0054 (15)	0.0037 (14)	0.0038 (13)
C3A	0.038 (2)	0.036 (2)	0.0220 (15)	0.0094 (16)	0.0015 (13)	0.0049 (14)
C4A	0.0330 (19)	0.0270 (18)	0.0241 (15)	0.0043 (14)	-0.0024 (13)	-0.0020 (13)
C5A	0.0229 (16)	0.0257 (17)	0.0246 (15)	0.0066 (13)	0.0028 (12)	0.0004 (12)
C6A	0.0228 (16)	0.0276 (17)	0.0219 (14)	0.0047 (13)	0.0006 (12)	0.0036 (12)
C7A	0.0224 (16)	0.0267 (18)	0.0215 (14)	-0.0003 (13)	0.0002 (12)	0.0021 (12)
C8A	0.0234 (17)	0.0210 (16)	0.0276 (15)	-0.0009 (13)	-0.0001 (12)	0.0021 (12)
C9A	0.0228 (16)	0.0268 (17)	0.0254 (15)	-0.0013 (13)	-0.0015 (12)	0.0015 (13)
C10A	0.0200 (16)	0.0336 (19)	0.0331 (17)	-0.0038 (14)	0.0013 (13)	-0.0002 (14)
C11A	0.0224 (16)	0.0240 (17)	0.0275 (15)	-0.0058 (13)	0.0061 (12)	-0.0001 (13)
C12A	0.0276 (17)	0.0210 (16)	0.0258 (15)	-0.0007 (13)	0.0027 (13)	0.0000 (12)
C13A	0.0227 (16)	0.0249 (17)	0.0254 (15)	-0.0016 (13)	0.0039 (12)	0.0010 (12)
C14A	0.0306 (18)	0.0267 (18)	0.0211 (14)	0.0041 (14)	0.0043 (12)	0.0020 (12)
C15A	0.0249 (17)	0.0290 (18)	0.0214 (14)	0.0026 (13)	0.0011 (12)	0.0009 (13)
C16A	0.0261 (17)	0.036 (2)	0.0228 (15)	0.0038 (14)	0.0034 (13)	0.0057 (13)
C17A	0.0334 (19)	0.040 (2)	0.0195 (14)	0.0060 (16)	0.0042 (13)	0.0005 (14)
C18A	0.0341 (19)	0.034 (2)	0.0252 (16)	0.0039 (15)	0.0037 (14)	-0.0045 (14)
C19A	0.0284 (18)	0.0314 (19)	0.0238 (15)	0.0036 (14)	0.0060 (13)	0.0022 (13)
C20A	0.0292 (18)	0.0310 (18)	0.0203 (14)	0.0050 (14)	0.0052 (12)	0.0011 (13)
C21A	0.035 (2)	0.0307 (19)	0.0229 (15)	0.0027 (15)	0.0045 (13)	-0.0037 (14)
C22A	0.0338 (19)	0.0231 (17)	0.0244 (15)	0.0008 (14)	0.0049 (13)	-0.0012 (12)
C23A	0.0334 (19)	0.0254 (17)	0.0329 (17)	0.0020 (15)	0.0147 (14)	0.0012 (14)
C24A	0.0241 (17)	0.0258 (18)	0.0389 (18)	0.0025 (14)	0.0045 (14)	0.0030 (14)
C25A	0.0294 (18)	0.0206 (16)	0.0285 (16)	0.0029 (14)	0.0027 (13)	0.0049 (13)
C26A	0.0235 (16)	0.0210 (17)	0.0282 (15)	0.0003 (13)	0.0051 (13)	0.0011 (13)
C27A	0.0253 (17)	0.0218 (16)	0.0281 (16)	0.0020 (13)	0.0033 (13)	-0.0004 (13)
C28A	0.0287 (17)	0.0241 (17)	0.0227 (14)	0.0011 (14)	0.0067 (12)	0.0007 (12)
C29A	0.119 (5)	0.066 (3)	0.027 (2)	-0.030 (3)	0.011 (2)	0.005 (2)
C30A	0.036 (2)	0.042 (2)	0.0353 (19)	-0.0046 (17)	-0.0044 (16)	-0.0043 (16)
C31A	0.049 (3)	0.046 (3)	0.047 (2)	-0.002 (2)	-0.017 (2)	0.000 (2)
C32A	0.073 (4)	0.094 (5)	0.135 (6)	0.008 (4)	-0.052 (4)	0.028 (5)
C33A	0.0304 (18)	0.0241 (17)	0.0285 (16)	0.0034 (14)	0.0034 (13)	0.0043 (13)
C34A	0.0307 (19)	0.0257 (18)	0.0351 (18)	0.0011 (15)	0.0023 (14)	0.0007 (14)
C35A	0.0308 (19)	0.0228 (17)	0.0327 (17)	-0.0005 (14)	0.0014 (14)	0.0020 (14)
C36A	0.041 (2)	0.035 (2)	0.0365 (19)	0.0097 (17)	0.0041 (16)	-0.0005 (16)
C37A	0.045 (2)	0.039 (2)	0.052 (2)	0.0129 (19)	0.017 (2)	0.0047 (19)
C38A	0.030 (2)	0.039 (2)	0.066 (3)	0.0053 (17)	0.0024 (19)	0.012 (2)
C39A	0.037 (2)	0.052 (3)	0.044 (2)	0.0019 (19)	-0.0063 (18)	0.0036 (19)
C40A	0.036 (2)	0.049 (3)	0.0348 (19)	0.0043 (18)	0.0003 (16)	-0.0030 (18)
C41A	0.026 (2)	0.064 (3)	0.040 (2)	0.0049 (19)	-0.0072 (16)	0.0056 (19)
C42A	0.031 (2)	0.033 (2)	0.0361 (18)	0.0053 (16)	0.0028 (15)	-0.0012 (15)
C43A	0.036 (2)	0.044 (2)	0.0338 (18)	0.0089 (18)	0.0039 (15)	-0.0041 (17)
C44A	0.076 (4)	0.057 (3)	0.049 (3)	0.004 (3)	0.031 (2)	0.006 (2)

C45A	0.0333 (19)	0.0297 (19)	0.0240 (15)	0.0063 (15)	-0.0011 (13)	0.0007 (13)
C46A	0.053 (3)	0.061 (3)	0.0273 (18)	0.026 (2)	0.0011 (17)	0.0036 (18)
C47A	0.049 (2)	0.055 (3)	0.0234 (17)	0.019 (2)	0.0064 (16)	0.0111 (17)
C48A	0.053 (3)	0.067 (3)	0.0286 (19)	-0.001 (2)	0.0096 (18)	0.0141 (19)
C49A	0.040 (3)	0.097 (4)	0.035 (2)	0.006 (3)	0.0115 (18)	0.019 (2)
C50A	0.053 (3)	0.082 (4)	0.060 (3)	0.027 (3)	0.007 (2)	0.004 (3)
C51A	0.068 (4)	0.056 (3)	0.075 (3)	0.023 (3)	0.007 (3)	0.000 (3)
C52A	0.044 (3)	0.060 (3)	0.057 (3)	0.012 (2)	0.002 (2)	0.001 (2)
C53A	0.087 (4)	0.063 (3)	0.0236 (18)	-0.026 (3)	0.011 (2)	0.0047 (19)
C54A	0.046 (2)	0.045 (2)	0.0312 (18)	0.0036 (19)	0.0042 (16)	-0.0079 (16)
C55A	0.057 (3)	0.037 (2)	0.048 (2)	0.013 (2)	0.018 (2)	0.0044 (19)
C56A	0.056 (3)	0.092 (4)	0.079 (4)	0.010 (3)	0.022 (3)	0.011 (3)
C57A	0.0343 (19)	0.038 (2)	0.0249 (15)	-0.0016 (16)	0.0021 (13)	-0.0023 (14)
C58A	0.043 (2)	0.057 (3)	0.0262 (17)	0.003 (2)	-0.0016 (15)	-0.0044 (17)
C59A	0.038 (2)	0.051 (2)	0.0246 (16)	-0.0087 (18)	-0.0034 (14)	-0.0052 (16)
C60A	0.041 (2)	0.061 (3)	0.042 (2)	-0.011 (2)	-0.0067 (17)	0.009 (2)
C61A	0.040 (3)	0.084 (4)	0.059 (3)	0.007 (3)	-0.011 (2)	0.007 (3)
C62A	0.047 (3)	0.101 (5)	0.044 (3)	-0.013 (3)	-0.006 (2)	0.001 (3)
C63A	0.069 (4)	0.092 (5)	0.046 (3)	-0.048 (3)	0.003 (2)	-0.007 (3)
C64A	0.063 (3)	0.048 (3)	0.045 (2)	-0.014 (2)	-0.005 (2)	-0.0042 (19)
C65A	0.040 (2)	0.043 (2)	0.053 (2)	0.0069 (18)	0.0228 (19)	0.0059 (18)
C66A	0.037 (2)	0.073 (3)	0.041 (2)	-0.015 (2)	-0.0050 (17)	0.010 (2)
C67A	0.049 (3)	0.057 (3)	0.045 (2)	-0.012 (2)	-0.0112 (19)	0.009 (2)
C68A	0.100 (4)	0.056 (3)	0.042 (2)	-0.011 (3)	-0.008 (3)	0.000 (2)
C69A	0.0291 (18)	0.0290 (18)	0.0306 (17)	0.0011 (15)	0.0042 (13)	-0.0018 (14)
C70A	0.0302 (19)	0.032 (2)	0.0411 (19)	0.0009 (15)	0.0042 (15)	-0.0011 (15)
C71A	0.033 (2)	0.038 (2)	0.0382 (19)	-0.0004 (17)	0.0006 (15)	-0.0072 (16)
C72A	0.045 (2)	0.051 (3)	0.046 (2)	0.006 (2)	0.0045 (18)	0.0000 (19)
C73A	0.047 (3)	0.064 (3)	0.053 (3)	0.010 (2)	-0.014 (2)	-0.004 (2)
C74A	0.036 (2)	0.074 (4)	0.076 (3)	0.018 (2)	-0.012 (2)	-0.025 (3)
C75A	0.035 (2)	0.099 (4)	0.055 (3)	0.006 (3)	0.003 (2)	-0.019 (3)
C76A	0.036 (2)	0.077 (3)	0.040 (2)	0.000 (2)	0.0025 (17)	-0.002 (2)
O1B	0.0579 (18)	0.0345 (15)	0.0222 (12)	0.0081 (13)	0.0111 (11)	-0.0023 (10)
O2B	0.0559 (18)	0.0388 (15)	0.0286 (12)	0.0081 (13)	0.0062 (11)	0.0121 (11)
O3B	0.061 (2)	0.086 (3)	0.0489 (18)	-0.0269 (19)	0.0013 (15)	-0.0055 (17)
O4B	0.058 (2)	0.124 (4)	0.0452 (18)	-0.002 (2)	0.0161 (15)	-0.020 (2)
O5B	0.0315 (14)	0.0574 (18)	0.0308 (13)	-0.0069 (13)	0.0056 (10)	0.0017 (12)
O6B	0.0348 (14)	0.0482 (17)	0.0304 (12)	-0.0007 (12)	-0.0034 (10)	-0.0035 (11)
O7B	0.105 (4)	0.153 (5)	0.063 (3)	0.058 (4)	-0.028 (2)	-0.006 (3)
O8B	0.126 (4)	0.063 (2)	0.0412 (18)	0.011 (2)	-0.0184 (19)	-0.0105 (17)
O9B	0.085 (2)	0.0377 (16)	0.0248 (12)	0.0183 (15)	0.0048 (13)	-0.0054 (11)
O10B	0.0358 (14)	0.0343 (14)	0.0266 (12)	0.0050 (11)	-0.0064 (10)	0.0053 (10)
O11B	0.082 (3)	0.104 (3)	0.061 (2)	0.013 (2)	-0.029 (2)	-0.035 (2)
O12B	0.056 (2)	0.069 (3)	0.111 (3)	0.0037 (19)	-0.041 (2)	-0.010 (2)
O13B	0.0230 (13)	0.0492 (17)	0.0305 (12)	-0.0025 (11)	-0.0046 (10)	0.0001 (11)
O14B	0.0362 (14)	0.0348 (14)	0.0294 (12)	0.0006 (11)	0.0091 (10)	0.0019 (10)
O15B	0.060 (2)	0.059 (2)	0.0388 (15)	-0.0052 (16)	0.0061 (13)	0.0166 (14)
O16B	0.0568 (19)	0.0422 (17)	0.0410 (15)	-0.0007 (14)	0.0209 (13)	0.0003 (13)
C1B	0.0244 (17)	0.0276 (18)	0.0230 (15)	-0.0043 (13)	0.0007 (12)	-0.0012 (13)

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C2B	0.0287 (18)	0.0316 (19)	0.0231 (15)	-0.0024 (14)	0.0009 (13)	-0.0037 (13)
C3B	0.0361 (19)	0.0346 (19)	0.0195 (14)	0.0010 (15)	0.0015 (13)	0.0025 (13)
C4B	0.0297 (18)	0.0307 (19)	0.0262 (16)	0.0014 (14)	0.0002 (13)	0.0056 (13)
C5B	0.0301 (18)	0.0283 (18)	0.0230 (15)	-0.0013 (14)	0.0013 (13)	0.0010 (13)
C6B	0.0239 (17)	0.0293 (18)	0.0223 (14)	0.0001 (13)	0.0018 (12)	0.0010 (12)
C7B	0.0288 (17)	0.0232 (17)	0.0258 (15)	0.0035 (14)	0.0016 (13)	0.0037 (13)
C8B	0.0318 (18)	0.0198 (16)	0.0259 (15)	0.0019 (14)	-0.0009 (13)	-0.0006 (12)
C9B	0.0284 (18)	0.0314 (19)	0.0291 (16)	-0.0007 (14)	0.0041 (13)	0.0031 (14)
C10B	0.0263 (18)	0.036 (2)	0.0384 (18)	-0.0064 (15)	0.0036 (14)	0.0036 (15)
C11B	0.0304 (19)	0.0296 (19)	0.0299 (17)	0.0032 (15)	-0.0041 (14)	-0.0017 (14)
C12B	0.0340 (19)	0.0199 (16)	0.0250 (15)	0.0016 (14)	0.0025 (13)	0.0006 (12)
C13B	0.0258 (17)	0.0226 (17)	0.0290 (16)	0.0022 (13)	0.0033 (13)	0.0008 (13)
C14B	0.0291 (17)	0.0204 (16)	0.0269 (15)	0.0040 (13)	0.0054 (13)	-0.0016 (12)
C15B	0.0244 (17)	0.0270 (18)	0.0245 (15)	-0.0012 (13)	-0.0006 (12)	-0.0011 (13)
C16B	0.039 (2)	0.0299 (19)	0.0255 (16)	0.0057 (16)	0.0045 (14)	-0.0062 (14)
C17B	0.039 (2)	0.038 (2)	0.0214 (15)	0.0036 (16)	-0.0011 (14)	-0.0004 (14)
C18B	0.0264 (17)	0.0289 (18)	0.0249 (15)	0.0014 (14)	-0.0031 (13)	0.0024 (13)
C19B	0.0243 (17)	0.0253 (17)	0.0229 (14)	0.0012 (13)	-0.0008 (12)	0.0008 (12)
C20B	0.0252 (17)	0.0290 (18)	0.0181 (14)	0.0043 (13)	0.0005 (12)	0.0009 (12)
C21B	0.0258 (17)	0.0240 (17)	0.0208 (14)	0.0016 (13)	-0.0001 (12)	-0.0008 (12)
C22B	0.0210 (16)	0.0240 (17)	0.0246 (15)	0.0065 (13)	-0.0005 (12)	-0.0012 (12)
C23B	0.0275 (18)	0.0266 (18)	0.0297 (16)	0.0028 (14)	-0.0055 (13)	-0.0018 (13)
C24B	0.0217 (17)	0.0324 (19)	0.0327 (17)	0.0006 (14)	0.0020 (13)	0.0008 (14)
C25B	0.0291 (18)	0.0289 (18)	0.0269 (16)	0.0061 (14)	0.0061 (13)	0.0043 (13)
C26B	0.0251 (17)	0.0212 (16)	0.0237 (14)	0.0027 (13)	-0.0019 (12)	0.0008 (12)
C27B	0.0202 (16)	0.0229 (17)	0.0283 (15)	0.0050 (13)	-0.0010 (12)	-0.0023 (12)
C28B	0.0312 (18)	0.0248 (17)	0.0207 (14)	0.0029 (14)	0.0032 (12)	-0.0004 (12)
C29B	0.078 (3)	0.063 (3)	0.0216 (17)	0.023 (3)	0.0114 (19)	-0.0030 (18)
C30B	0.049 (2)	0.042 (2)	0.0313 (18)	0.0049 (19)	0.0023 (16)	0.0118 (16)
C31B	0.056 (3)	0.037 (2)	0.037 (2)	-0.0040 (19)	0.0027 (18)	0.0060 (17)
C32B	0.062 (4)	0.138 (7)	0.071 (4)	-0.001 (4)	0.020 (3)	-0.021 (4)
C33B	0.0286 (18)	0.0279 (18)	0.0341 (17)	0.0029 (14)	-0.0032 (14)	0.0055 (14)
C34B	0.034 (2)	0.043 (2)	0.0364 (19)	0.0056 (17)	-0.0036 (15)	0.0059 (16)
C35B	0.0321 (19)	0.036 (2)	0.0338 (18)	-0.0001 (16)	-0.0053 (14)	0.0072 (15)
C36B	0.038 (2)	0.033 (2)	0.075 (3)	0.0004 (18)	-0.007 (2)	-0.008 (2)
C37B	0.042 (2)	0.039 (2)	0.070 (3)	0.0081 (19)	-0.003 (2)	-0.008 (2)
C38B	0.032 (2)	0.051 (3)	0.053 (2)	-0.0052 (19)	-0.0086 (18)	0.002 (2)
C39B	0.050 (3)	0.047 (3)	0.063 (3)	-0.008 (2)	-0.016 (2)	-0.008 (2)
C40B	0.044 (2)	0.044 (2)	0.050 (2)	0.0033 (19)	-0.0125 (19)	-0.0105 (19)
C41B	0.036 (2)	0.076 (3)	0.038 (2)	-0.008 (2)	0.0077 (17)	0.001 (2)
C42B	0.034 (2)	0.073 (3)	0.045 (2)	0.007 (2)	-0.0016 (18)	-0.011 (2)
C43B	0.055 (3)	0.073 (4)	0.048 (3)	-0.002 (3)	-0.010 (2)	-0.002 (2)
C44B	0.216 (10)	0.112 (6)	0.036 (3)	0.008 (6)	-0.010 (4)	-0.014 (3)
C45B	0.0309 (19)	0.0288 (18)	0.0307 (17)	0.0034 (15)	0.0067 (14)	0.0043 (14)
C46B	0.032 (2)	0.031 (2)	0.0394 (19)	0.0048 (16)	0.0057 (15)	0.0060 (16)
C47B	0.0290 (19)	0.038 (2)	0.0408 (19)	0.0105 (16)	0.0051 (15)	0.0120 (16)
C48B	0.044 (3)	0.066 (3)	0.046 (2)	0.006 (2)	0.0087 (19)	0.002 (2)
C49B	0.037 (2)	0.091 (4)	0.061 (3)	0.006 (3)	0.019 (2)	0.008 (3)
C50B	0.039 (3)	0.066 (3)	0.071 (3)	-0.008 (2)	0.000 (2)	0.012 (3)

C51B	0.057 (3)	0.051 (3)	0.066 (3)	0.002 (2)	-0.008 (2)	0.001 (2)
C52B	0.043 (2)	0.044 (2)	0.055 (2)	0.010 (2)	0.0054 (19)	-0.003 (2)
C53B	0.207 (8)	0.082 (4)	0.033 (2)	0.079 (5)	0.019 (3)	-0.009 (3)
C54B	0.048 (2)	0.042 (2)	0.0324 (19)	0.0068 (19)	-0.0085 (17)	0.0043 (17)
C55B	0.059 (3)	0.052 (3)	0.053 (3)	0.002 (2)	-0.024 (2)	-0.002 (2)
C56B	0.082 (5)	0.120 (7)	0.207 (10)	-0.015 (5)	-0.085 (6)	-0.030 (7)
C57B	0.0229 (17)	0.0294 (18)	0.0253 (15)	0.0029 (14)	0.0027 (12)	0.0003 (13)
C58B	0.0287 (18)	0.0253 (18)	0.0317 (17)	0.0002 (14)	-0.0011 (14)	0.0003 (14)
C59B	0.0292 (19)	0.0248 (18)	0.0327 (17)	-0.0002 (14)	0.0003 (14)	-0.0031 (14)
C60B	0.038 (2)	0.042 (2)	0.0345 (19)	-0.0067 (18)	-0.0009 (16)	-0.0024 (16)
C61B	0.038 (2)	0.047 (3)	0.049 (2)	-0.0115 (19)	0.0128 (18)	-0.0028 (19)
C62B	0.035 (2)	0.042 (2)	0.060 (3)	-0.0083 (19)	-0.0028 (19)	-0.008 (2)
C63B	0.043 (2)	0.054 (3)	0.042 (2)	-0.009 (2)	-0.0055 (18)	-0.0066 (19)
C64B	0.037 (2)	0.048 (2)	0.0315 (18)	-0.0095 (18)	0.0041 (15)	-0.0007 (16)
C65B	0.027 (2)	0.064 (3)	0.045 (2)	-0.0070 (19)	-0.0034 (17)	-0.008 (2)
C66B	0.034 (2)	0.033 (2)	0.0377 (19)	-0.0012 (16)	0.0069 (15)	0.0074 (15)
C67B	0.034 (2)	0.040 (2)	0.039 (2)	-0.0075 (18)	0.0011 (16)	0.0032 (17)
C68B	0.082 (4)	0.059 (3)	0.049 (3)	-0.005 (3)	0.032 (2)	-0.007 (2)
C69B	0.0344 (19)	0.0293 (18)	0.0233 (15)	-0.0070 (15)	0.0028 (13)	-0.0023 (13)
C70B	0.062 (3)	0.050 (3)	0.0260 (18)	-0.027 (2)	0.0005 (17)	-0.0021 (17)
C71B	0.051 (3)	0.058 (3)	0.0240 (17)	-0.021 (2)	0.0019 (16)	-0.0103 (17)
C72B	0.062 (3)	0.058 (3)	0.048 (2)	-0.024 (2)	-0.009 (2)	0.008 (2)
C73B	0.077 (4)	0.075 (4)	0.068 (3)	-0.036 (3)	-0.009 (3)	0.014 (3)
C74B	0.068 (4)	0.100 (5)	0.057 (3)	-0.050 (4)	0.002 (3)	0.003 (3)
C75B	0.041 (3)	0.119 (5)	0.040 (2)	-0.006 (3)	0.0136 (19)	-0.019 (3)
C76B	0.064 (3)	0.067 (3)	0.040 (2)	-0.003 (3)	0.011 (2)	-0.019 (2)
O1C	0.0572 (18)	0.0312 (14)	0.0275 (12)	-0.0055 (13)	0.0042 (11)	0.0070 (10)
O2C	0.0383 (15)	0.0328 (14)	0.0307 (12)	-0.0051 (11)	-0.0053 (10)	-0.0027 (10)
O3C	0.080 (3)	0.100 (3)	0.057 (2)	-0.018 (2)	-0.0243 (19)	0.039 (2)
O4C	0.056 (2)	0.059 (2)	0.077 (2)	0.0070 (17)	-0.0271 (18)	0.0057 (18)
O5C	0.0256 (13)	0.0475 (16)	0.0311 (12)	0.0027 (11)	-0.0069 (10)	0.0063 (11)
O6C	0.0301 (13)	0.0284 (13)	0.0332 (12)	-0.0001 (10)	0.0062 (10)	-0.0004 (10)
O7C	0.060 (2)	0.070 (2)	0.067 (2)	0.0127 (18)	-0.0038 (16)	-0.0343 (19)
O8C	0.095 (3)	0.049 (2)	0.0506 (18)	0.0105 (19)	0.0369 (18)	0.0010 (15)
O9C	0.0628 (19)	0.0354 (15)	0.0214 (12)	-0.0171 (14)	0.0027 (12)	0.0041 (10)
C54C	0.083 (4)	0.043 (3)	0.066 (3)	-0.004 (3)	0.019 (3)	-0.012 (2)
O11C	0.174 (6)	0.236 (9)	0.093 (4)	-0.003 (6)	0.066 (4)	-0.024 (5)
O12C	0.113 (4)	0.074 (3)	0.074 (3)	0.001 (3)	-0.023 (2)	-0.020 (2)
O13C	0.0360 (15)	0.0466 (17)	0.0351 (13)	0.0047 (13)	0.0113 (11)	-0.0010 (12)
O14C	0.0296 (14)	0.0410 (16)	0.0360 (13)	-0.0049 (12)	-0.0040 (10)	0.0078 (11)
O15C	0.100 (3)	0.148 (5)	0.062 (2)	-0.074 (3)	-0.025 (2)	0.009 (3)
O16C	0.0499 (18)	0.066 (2)	0.0401 (15)	-0.0125 (16)	-0.0094 (13)	-0.0007 (14)
C1C	0.0264 (17)	0.0260 (17)	0.0273 (16)	0.0004 (14)	0.0042 (13)	0.0008 (13)
C2C	0.0296 (18)	0.0289 (18)	0.0275 (16)	-0.0032 (14)	0.0037 (13)	0.0049 (13)
C3C	0.033 (2)	0.036 (2)	0.0262 (16)	-0.0006 (16)	0.0004 (14)	0.0037 (14)
C4C	0.0271 (18)	0.0296 (18)	0.0268 (16)	-0.0032 (14)	0.0004 (13)	0.0005 (13)
C5C	0.0217 (16)	0.0249 (17)	0.0258 (15)	-0.0005 (13)	0.0010 (12)	0.0043 (12)
C6C	0.0220 (16)	0.0304 (18)	0.0243 (15)	-0.0021 (13)	-0.0002 (12)	0.0032 (13)
C7C	0.0245 (17)	0.0264 (17)	0.0234 (15)	-0.0051 (13)	-0.0020 (12)	0.0046 (13)

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C8C	0.0271 (17)	0.0213 (16)	0.0262 (15)	-0.0043 (13)	-0.0022 (13)	0.0049 (12)
C9C	0.0253 (17)	0.0267 (18)	0.0279 (16)	-0.0032 (14)	-0.0043 (13)	0.0049 (13)
C10C	0.0230 (17)	0.0271 (18)	0.0344 (17)	-0.0030 (14)	-0.0011 (13)	0.0023 (14)
C11C	0.0265 (17)	0.0229 (17)	0.0297 (16)	-0.0048 (14)	0.0039 (13)	0.0025 (13)
C12C	0.0253 (16)	0.0193 (16)	0.0263 (15)	-0.0042 (13)	-0.0024 (12)	0.0038 (12)
C13C	0.0183 (15)	0.0239 (17)	0.0290 (15)	-0.0022 (13)	-0.0019 (12)	0.0041 (13)
C14C	0.0302 (18)	0.0232 (17)	0.0230 (14)	-0.0017 (14)	0.0030 (12)	0.0039 (12)
C15C	0.0268 (17)	0.0265 (18)	0.0272 (16)	-0.0008 (14)	-0.0029 (13)	0.0011 (13)
C16C	0.0312 (19)	0.0306 (19)	0.0263 (16)	-0.0070 (15)	0.0002 (13)	0.0012 (14)
C17C	0.045 (2)	0.037 (2)	0.0232 (16)	-0.0068 (17)	0.0013 (14)	-0.0013 (14)
C18C	0.043 (2)	0.0281 (19)	0.0284 (17)	-0.0066 (16)	0.0000 (15)	-0.0040 (14)
C19C	0.0318 (19)	0.0278 (18)	0.0261 (16)	-0.0063 (15)	-0.0014 (13)	-0.0003 (13)
C20C	0.0276 (18)	0.0296 (18)	0.0229 (15)	-0.0007 (14)	0.0029 (13)	0.0014 (13)
C21C	0.039 (2)	0.0220 (17)	0.0262 (16)	-0.0044 (15)	0.0030 (14)	-0.0016 (13)
C22C	0.0317 (18)	0.0188 (16)	0.0323 (17)	-0.0022 (14)	0.0027 (14)	0.0007 (13)
C23C	0.0314 (19)	0.0246 (17)	0.0346 (17)	-0.0001 (14)	0.0076 (14)	0.0009 (14)
C24C	0.0250 (18)	0.0311 (19)	0.0403 (19)	0.0030 (15)	0.0025 (14)	0.0021 (15)
C25C	0.0308 (19)	0.0270 (18)	0.0309 (17)	0.0015 (15)	-0.0015 (14)	0.0029 (14)
C26C	0.0271 (17)	0.0209 (16)	0.0279 (15)	-0.0036 (13)	0.0043 (13)	0.0027 (12)
C27C	0.0302 (18)	0.0203 (17)	0.0310 (16)	-0.0016 (14)	0.0008 (13)	0.0021 (13)
C28C	0.0312 (18)	0.0232 (17)	0.0275 (16)	-0.0035 (14)	0.0049 (13)	0.0052 (13)
C29C	0.087 (4)	0.055 (3)	0.033 (2)	-0.010 (3)	0.000 (2)	0.011 (2)
C30C	0.037 (2)	0.035 (2)	0.041 (2)	-0.0070 (17)	-0.0123 (16)	0.0038 (16)
C31C	0.059 (3)	0.041 (2)	0.046 (2)	-0.010 (2)	-0.026 (2)	0.0041 (19)
C32C	0.088 (5)	0.083 (5)	0.137 (6)	0.015 (4)	-0.067 (5)	0.019 (4)
C33C	0.0271 (18)	0.0292 (19)	0.0294 (16)	-0.0023 (14)	0.0014 (13)	0.0042 (14)
C34C	0.0303 (19)	0.0268 (18)	0.0364 (18)	-0.0017 (15)	-0.0018 (14)	0.0052 (14)
C35C	0.0318 (19)	0.0267 (19)	0.0358 (18)	0.0011 (15)	-0.0009 (15)	0.0068 (15)
C36C	0.062 (3)	0.058 (3)	0.039 (2)	0.024 (2)	-0.002 (2)	-0.001 (2)
C37C	0.070 (3)	0.064 (3)	0.056 (3)	0.035 (3)	0.019 (2)	0.003 (2)
C38C	0.038 (2)	0.051 (3)	0.071 (3)	0.014 (2)	0.010 (2)	0.020 (2)
C39C	0.042 (3)	0.050 (3)	0.061 (3)	0.003 (2)	-0.016 (2)	0.007 (2)
C40C	0.036 (2)	0.050 (3)	0.044 (2)	0.0037 (19)	-0.0004 (17)	-0.0061 (18)
C41C	0.033 (2)	0.056 (3)	0.047 (2)	0.0044 (19)	-0.0050 (17)	0.008 (2)
C42C	0.034 (2)	0.0294 (19)	0.044 (2)	0.0025 (16)	0.0022 (16)	-0.0036 (16)
C43C	0.040 (2)	0.047 (3)	0.046 (2)	0.0157 (19)	-0.0042 (18)	-0.008 (2)
C44C	0.118 (6)	0.089 (5)	0.061 (3)	0.037 (4)	0.043 (3)	0.013 (3)
C45C	0.0332 (19)	0.033 (2)	0.0300 (17)	0.0035 (15)	-0.0012 (14)	0.0054 (14)
C46C	0.049 (3)	0.059 (3)	0.0286 (18)	0.021 (2)	-0.0040 (16)	0.0050 (18)
C47C	0.050 (3)	0.061 (3)	0.0244 (17)	0.017 (2)	-0.0015 (16)	0.0110 (17)
C48C	0.049 (3)	0.057 (3)	0.056 (3)	0.016 (2)	-0.009 (2)	0.000 (2)
C49C	0.059 (3)	0.066 (4)	0.069 (3)	0.025 (3)	-0.004 (3)	-0.006 (3)
C50C	0.047 (3)	0.083 (4)	0.060 (3)	0.025 (3)	0.004 (2)	0.010 (3)
C51C	0.040 (2)	0.081 (4)	0.037 (2)	0.004 (2)	0.0116 (17)	0.013 (2)
C52C	0.054 (3)	0.063 (3)	0.038 (2)	0.006 (2)	0.0077 (19)	0.016 (2)
C53C	0.128 (5)	0.068 (3)	0.0209 (19)	-0.056 (4)	0.007 (2)	-0.001 (2)
O10C	0.077 (2)	0.0334 (15)	0.0348 (14)	-0.0098 (15)	0.0110 (13)	-0.0101 (12)
C55C	0.095 (5)	0.073 (4)	0.065 (3)	0.001 (4)	0.028 (3)	-0.016 (3)
C56C	0.162 (8)	0.145 (8)	0.074 (5)	-0.031 (7)	-0.012 (5)	-0.021 (5)

C57C	0.036 (2)	0.0266 (18)	0.0334 (17)	-0.0039 (15)	-0.0011 (14)	0.0003 (14)
C58C	0.049 (2)	0.036 (2)	0.0380 (19)	-0.0118 (18)	-0.0099 (17)	0.0018 (16)
C59C	0.055 (3)	0.031 (2)	0.051 (2)	-0.0112 (19)	-0.0189 (19)	-0.0037 (18)
C60C	0.040 (3)	0.044 (3)	0.090 (4)	-0.002 (2)	-0.019 (2)	0.018 (3)
C61C	0.050 (3)	0.045 (3)	0.115 (5)	-0.004 (2)	-0.017 (3)	0.008 (3)
C62C	0.056 (3)	0.054 (3)	0.132 (6)	0.004 (3)	-0.041 (4)	-0.022 (4)
C63C	0.090 (5)	0.077 (4)	0.074 (4)	0.025 (4)	-0.051 (3)	-0.016 (3)
C64C	0.083 (4)	0.062 (3)	0.050 (3)	-0.003 (3)	-0.031 (2)	0.000 (2)
C65C	0.036 (2)	0.066 (3)	0.054 (2)	0.014 (2)	0.0203 (19)	0.005 (2)
C66C	0.064 (3)	0.129 (6)	0.045 (3)	-0.051 (4)	-0.012 (2)	0.016 (3)
C67C	0.050 (3)	0.092 (4)	0.044 (2)	-0.029 (3)	-0.008 (2)	0.000 (2)
C68C	0.083 (4)	0.081 (4)	0.035 (2)	-0.004 (3)	-0.012 (2)	0.001 (2)
C69C	0.0282 (18)	0.0283 (18)	0.0371 (18)	-0.0046 (15)	0.0087 (14)	-0.0032 (15)
C70C	0.032 (2)	0.0272 (19)	0.047 (2)	-0.0064 (16)	0.0067 (16)	-0.0055 (16)
C71C	0.033 (2)	0.031 (2)	0.071 (3)	-0.0090 (17)	0.0081 (19)	-0.010 (2)
C72C	0.038 (3)	0.051 (3)	0.113 (4)	-0.011 (2)	-0.007 (3)	0.018 (3)
C73C	0.048 (4)	0.059 (4)	0.221 (9)	-0.008 (3)	-0.034 (5)	0.037 (5)
C74C	0.031 (3)	0.065 (5)	0.301 (14)	-0.002 (3)	0.023 (6)	-0.009 (7)
C75C	0.052 (4)	0.089 (5)	0.188 (8)	-0.013 (4)	0.060 (5)	-0.021 (6)
C76C	0.047 (3)	0.067 (3)	0.091 (4)	-0.019 (3)	0.026 (3)	-0.011 (3)
O1D	0.0489 (16)	0.0317 (14)	0.0235 (11)	0.0008 (12)	0.0046 (10)	-0.0070 (10)
O2D	0.0319 (14)	0.0323 (14)	0.0299 (12)	0.0030 (11)	-0.0024 (10)	0.0057 (10)
O3D	0.072 (2)	0.092 (3)	0.0454 (18)	0.014 (2)	-0.0192 (17)	-0.0190 (19)
O4D	0.048 (2)	0.062 (2)	0.070 (2)	-0.0097 (16)	-0.0229 (16)	-0.0108 (17)
O5D	0.0229 (12)	0.0432 (15)	0.0266 (11)	0.0001 (11)	-0.0054 (9)	-0.0046 (10)
O6D	0.0314 (13)	0.0247 (12)	0.0291 (12)	-0.0022 (10)	0.0083 (10)	-0.0040 (9)
O7D	0.066 (2)	0.0456 (19)	0.0582 (19)	-0.0045 (16)	0.0135 (16)	0.0159 (15)
O8D	0.068 (2)	0.0372 (16)	0.0415 (15)	-0.0041 (15)	0.0246 (14)	-0.0015 (12)
O9D	0.068 (2)	0.0470 (18)	0.0229 (13)	0.0121 (15)	0.0080 (12)	-0.0029 (12)
O10D	0.066 (2)	0.0449 (17)	0.0290 (13)	-0.0021 (15)	0.0100 (12)	0.0124 (12)
O11D	0.129 (4)	0.209 (7)	0.051 (2)	-0.071 (4)	0.021 (2)	0.029 (3)
O12D	0.073 (3)	0.113 (3)	0.0442 (18)	-0.001 (2)	-0.0042 (17)	0.015 (2)
O13D	0.0304 (13)	0.0445 (15)	0.0282 (11)	-0.0058 (11)	0.0070 (10)	0.0016 (11)
O14D	0.0252 (12)	0.0397 (14)	0.0230 (10)	-0.0041 (11)	-0.0026 (9)	-0.0024 (10)
O15D	0.058 (2)	0.146 (4)	0.0466 (18)	0.047 (2)	-0.0134 (15)	0.001 (2)
O16D	0.0404 (15)	0.0494 (17)	0.0273 (12)	0.0010 (12)	-0.0043 (11)	0.0002 (11)
C1D	0.0221 (16)	0.0267 (17)	0.0237 (15)	-0.0009 (13)	0.0016 (12)	0.0013 (13)
C2D	0.0270 (17)	0.0270 (17)	0.0229 (15)	-0.0047 (14)	0.0023 (12)	-0.0043 (13)
C3D	0.0300 (18)	0.035 (2)	0.0195 (14)	-0.0033 (15)	0.0002 (12)	-0.0009 (13)
C4D	0.0241 (17)	0.0290 (18)	0.0243 (15)	0.0009 (14)	-0.0033 (13)	0.0034 (13)
C5D	0.0214 (16)	0.0286 (18)	0.0232 (15)	0.0005 (14)	-0.0016 (12)	-0.0041 (13)
C6D	0.0239 (16)	0.0265 (17)	0.0211 (14)	-0.0002 (13)	0.0005 (12)	-0.0012 (12)
C7D	0.0233 (16)	0.0225 (16)	0.0246 (15)	0.0000 (13)	-0.0001 (12)	-0.0008 (12)
C8D	0.0224 (16)	0.0231 (16)	0.0221 (14)	0.0048 (13)	0.0009 (12)	-0.0028 (12)
C9D	0.0261 (17)	0.0245 (17)	0.0261 (15)	0.0045 (13)	-0.0028 (13)	-0.0040 (12)
C10D	0.0200 (16)	0.0292 (18)	0.0305 (16)	0.0040 (14)	-0.0009 (13)	-0.0034 (14)
C11D	0.0268 (17)	0.0197 (16)	0.0283 (16)	0.0042 (13)	0.0017 (13)	-0.0026 (12)
C12D	0.0268 (17)	0.0228 (16)	0.0243 (15)	0.0026 (13)	-0.0024 (12)	-0.0055 (12)
C13D	0.0219 (16)	0.0238 (17)	0.0270 (15)	0.0026 (13)	-0.0016 (12)	-0.0028 (12)

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C14D	0.0258 (17)	0.0319 (19)	0.0230 (15)	0.0014 (14)	-0.0027 (12)	-0.0063 (13)
C15D	0.0230 (17)	0.037 (2)	0.0208 (14)	-0.0003 (14)	-0.0047 (12)	-0.0010 (13)
C16D	0.035 (2)	0.042 (2)	0.0217 (15)	0.0047 (16)	-0.0028 (14)	-0.0036 (14)
C17D	0.048 (2)	0.047 (2)	0.0184 (15)	0.0031 (18)	0.0027 (15)	0.0019 (15)
C18D	0.039 (2)	0.041 (2)	0.0265 (17)	-0.0034 (17)	-0.0027 (15)	0.0056 (15)
C19D	0.0260 (17)	0.0311 (19)	0.0254 (15)	-0.0019 (14)	-0.0033 (13)	-0.0017 (13)
C20D	0.0233 (17)	0.0368 (19)	0.0183 (14)	-0.0016 (14)	0.0002 (12)	-0.0001 (13)
C21D	0.0356 (19)	0.0293 (19)	0.0223 (15)	-0.0037 (15)	-0.0031 (13)	0.0020 (13)
C22D	0.0327 (18)	0.0239 (17)	0.0220 (14)	-0.0018 (14)	-0.0016 (13)	0.0029 (12)
C23D	0.0323 (18)	0.0238 (17)	0.0258 (15)	-0.0012 (14)	0.0070 (13)	0.0009 (13)
C24D	0.0238 (17)	0.0281 (18)	0.0285 (15)	-0.0029 (14)	-0.0008 (13)	-0.0016 (14)
C25D	0.0265 (17)	0.0207 (16)	0.0248 (15)	0.0012 (13)	0.0007 (12)	-0.0010 (12)
C26D	0.0277 (18)	0.0223 (17)	0.0223 (14)	-0.0032 (13)	0.0015 (12)	0.0006 (12)
C27D	0.0234 (17)	0.0226 (17)	0.0296 (16)	-0.0018 (13)	0.0007 (13)	0.0012 (13)
C28D	0.0268 (17)	0.0235 (17)	0.0237 (15)	0.0009 (13)	0.0036 (12)	0.0004 (12)
C29D	0.060 (3)	0.043 (2)	0.0259 (17)	0.003 (2)	-0.0002 (17)	-0.0114 (16)
C30D	0.034 (2)	0.038 (2)	0.0341 (18)	0.0073 (16)	-0.0109 (15)	0.0002 (15)
C31D	0.049 (3)	0.035 (2)	0.044 (2)	0.0111 (19)	-0.0204 (19)	-0.0037 (17)
C32D	0.093 (5)	0.069 (4)	0.109 (5)	-0.023 (3)	-0.054 (4)	-0.012 (4)
C33D	0.0239 (17)	0.028 (2)	0.0289 (17)	0.0025 (14)	0.0026 (13)	-0.0038 (13)
C34D	0.0234 (17)	0.033 (2)	0.0349 (17)	0.0020 (14)	-0.0003 (14)	-0.0050 (15)
C35D	0.031 (2)	0.0220 (18)	0.0370 (18)	-0.0012 (15)	0.0045 (15)	-0.0025 (14)
C36D	0.047 (2)	0.040 (2)	0.039 (2)	-0.0071 (18)	0.0044 (17)	-0.0002 (17)
C37D	0.056 (3)	0.042 (2)	0.057 (3)	-0.020 (2)	0.016 (2)	-0.004 (2)
C38D	0.032 (2)	0.044 (2)	0.069 (3)	-0.0080 (18)	0.005 (2)	-0.019 (2)
C39D	0.035 (2)	0.058 (3)	0.050 (2)	0.003 (2)	-0.0036 (19)	-0.007 (2)
C40D	0.037 (2)	0.045 (2)	0.0376 (19)	-0.0045 (18)	-0.0005 (16)	0.0009 (17)
C41D	0.035 (2)	0.055 (3)	0.037 (2)	-0.0089 (18)	-0.0090 (16)	-0.0075 (18)
C42D	0.033 (2)	0.0240 (18)	0.0389 (19)	-0.0015 (15)	-0.0015 (15)	0.0012 (14)
C43D	0.042 (2)	0.036 (2)	0.0335 (18)	-0.0058 (17)	0.0001 (16)	0.0018 (16)
C44D	0.098 (4)	0.063 (3)	0.051 (3)	-0.007 (3)	0.046 (3)	-0.003 (2)
C45D	0.0308 (19)	0.036 (2)	0.0248 (16)	-0.0055 (15)	-0.0026 (13)	-0.0015 (14)
C46D	0.047 (3)	0.064 (3)	0.0298 (19)	-0.022 (2)	-0.0068 (16)	-0.0006 (18)
C47D	0.047 (3)	0.066 (3)	0.0231 (17)	-0.019 (2)	0.0017 (16)	-0.0126 (18)
C48D	0.050 (3)	0.070 (3)	0.044 (2)	-0.014 (2)	-0.006 (2)	0.001 (2)
C49D	0.061 (3)	0.068 (4)	0.063 (3)	-0.026 (3)	-0.003 (2)	0.007 (3)
C50D	0.051 (3)	0.088 (4)	0.046 (3)	-0.028 (3)	0.005 (2)	-0.007 (3)
C51D	0.038 (2)	0.091 (4)	0.035 (2)	-0.016 (2)	0.0099 (17)	-0.019 (2)
C52D	0.051 (3)	0.067 (3)	0.032 (2)	-0.005 (2)	0.0058 (18)	-0.0172 (19)
C53D	0.115 (5)	0.083 (4)	0.0167 (18)	0.048 (3)	0.010 (2)	-0.002 (2)
C54D	0.066 (3)	0.056 (3)	0.052 (3)	-0.018 (3)	0.002 (2)	0.012 (2)
C55D	0.079 (4)	0.057 (3)	0.043 (2)	-0.010 (3)	0.013 (2)	0.013 (2)
C56D	0.133 (7)	0.141 (7)	0.054 (3)	0.009 (5)	-0.038 (4)	-0.003 (4)
C57D	0.035 (2)	0.036 (2)	0.0270 (16)	0.0012 (16)	-0.0061 (14)	0.0039 (14)
C58D	0.039 (2)	0.078 (3)	0.039 (2)	0.000 (2)	-0.0046 (17)	0.018 (2)
C59D	0.049 (2)	0.046 (2)	0.0364 (19)	0.0013 (19)	-0.0108 (17)	0.0086 (17)
C60D	0.056 (3)	0.077 (4)	0.084 (4)	0.013 (3)	-0.028 (3)	-0.038 (3)
C61D	0.058 (4)	0.143 (7)	0.096 (5)	0.032 (4)	-0.011 (3)	-0.041 (5)
C62D	0.047 (3)	0.118 (6)	0.065 (3)	-0.014 (3)	-0.017 (2)	0.003 (3)

C63D	0.087 (4)	0.076 (4)	0.064 (3)	-0.024 (3)	-0.038 (3)	0.002 (3)
C64D	0.069 (3)	0.073 (4)	0.043 (2)	0.010 (3)	-0.018 (2)	-0.010 (2)
C65D	0.037 (2)	0.037 (2)	0.0407 (19)	-0.0032 (17)	0.0104 (16)	-0.0077 (16)
C66D	0.035 (2)	0.062 (3)	0.0344 (18)	0.0153 (19)	-0.0014 (15)	-0.0046 (18)
C67D	0.042 (2)	0.071 (3)	0.0325 (19)	0.010 (2)	-0.0041 (17)	0.0015 (19)
C68D	0.059 (3)	0.058 (3)	0.034 (2)	-0.007 (2)	-0.0142 (19)	0.0001 (19)
C69D	0.0284 (18)	0.0288 (18)	0.0337 (17)	-0.0024 (15)	0.0088 (14)	0.0054 (14)
C70D	0.036 (2)	0.036 (2)	0.046 (2)	0.0039 (17)	0.0048 (17)	0.0035 (17)
C71D	0.029 (2)	0.033 (2)	0.075 (3)	0.0055 (17)	0.0044 (19)	0.011 (2)
C72D	0.046 (3)	0.093 (5)	0.094 (4)	0.018 (3)	0.025 (3)	0.043 (4)
C73D	0.046 (4)	0.113 (7)	0.185 (9)	0.029 (4)	0.048 (5)	0.078 (7)
C74D	0.047 (4)	0.083 (6)	0.256 (13)	-0.013 (4)	0.005 (6)	0.038 (7)
C75D	0.047 (3)	0.058 (4)	0.207 (9)	-0.004 (3)	-0.024 (5)	-0.017 (5)
C76D	0.037 (3)	0.052 (3)	0.118 (5)	0.005 (2)	-0.005 (3)	-0.020 (3)

Geometric parameters (Å, °)

O1A—C2A	1.373 (4)	O1C—C2C	1.381 (4)
O1A—C29A	1.430 (5)	O1C—C29C	1.439 (5)
O2A—C4A	1.398 (4)	O2C—C4C	1.394 (4)
O2A—C30A	1.425 (5)	O2C—C30C	1.431 (5)
O3A—C31A	1.196 (6)	O3C—C31C	1.177 (6)
O4A—C31A	1.341 (6)	O4C—C31C	1.354 (6)
O4A—C32A	1.452 (7)	O4C—C32C	1.454 (6)
O5A—C9A	1.375 (4)	O5C—C9C	1.375 (4)
O5A—C41A	1.412 (4)	O5C—C41C	1.433 (5)
O6A—C11A	1.393 (4)	O6C—C11C	1.388 (4)
O6A—C42A	1.415 (4)	O6C—C42C	1.425 (5)
O7A—C43A	1.209 (5)	O7C—C43C	1.201 (5)
O8A—C43A	1.316 (5)	O8C—C43C	1.333 (6)
O8A—C44A	1.443 (5)	O8C—C44C	1.458 (6)
O9A—C16A	1.362 (4)	O9C—C16C	1.374 (4)
O9A—C53A	1.412 (4)	O9C—C53C	1.403 (5)
O10A—C18A	1.383 (5)	C54C—C55C	1.428 (8)
O10A—C54A	1.426 (4)	C54C—O10C	1.444 (6)
O11A—C55A	1.197 (6)	C54C—H54E	0.9900
O12A—C55A	1.289 (5)	C54C—H54F	0.9900
O12A—C56A	1.454 (6)	O11C—C55C	1.166 (7)
O13A—C23A	1.375 (4)	O12C—C55C	1.338 (8)
O13A—C65A	1.426 (5)	O12C—C56C	1.536 (8)
O14A—C25A	1.382 (4)	O13C—C23C	1.373 (4)
O14A—C66A	1.396 (5)	O13C—C65C	1.427 (5)
O15A—C67A	1.196 (6)	O14C—C25C	1.399 (4)
O16A—C67A	1.314 (5)	O14C—C66C	1.402 (6)
O16A—C68A	1.441 (5)	O15C—C67C	1.193 (6)
C1A—C6A	1.393 (5)	O16C—C67C	1.337 (6)
C1A—C2A	1.404 (4)	O16C—C68C	1.455 (5)
C1A—C28A	1.529 (5)	C1C—C6C	1.393 (5)
C2A—C3A	1.377 (5)	C1C—C2C	1.403 (5)

supplementary materials

C3A—C4A	1.392 (5)	C1C—C28C	1.517 (5)
C3A—H3A	0.9500	C2C—C3C	1.372 (5)
C4A—C5A	1.395 (4)	C3C—C4C	1.390 (5)
C5A—C6A	1.393 (5)	C3C—H3C	0.9500
C5A—C7A	1.524 (5)	C4C—C5C	1.397 (4)
C6A—H6A	0.9500	C5C—C6C	1.382 (5)
C7A—C8A	1.528 (4)	C5C—C7C	1.534 (4)
C7A—C33A	1.553 (5)	C6C—H6C	0.9500
C7A—H7A	1.0000	C7C—C8C	1.518 (5)
C8A—C13A	1.393 (4)	C7C—C33C	1.532 (5)
C8A—C9A	1.401 (5)	C7C—H7C	1.0000
C9A—C10A	1.391 (5)	C8C—C13C	1.388 (4)
C10A—C11A	1.388 (5)	C8C—C9C	1.405 (5)
C10A—H10A	0.9500	C9C—C10C	1.381 (5)
C11A—C12A	1.390 (5)	C10C—C11C	1.388 (5)
C12A—C13A	1.409 (4)	C10C—H10C	0.9500
C12A—C14A	1.511 (4)	C11C—C12C	1.389 (5)
C13A—H13A	0.9500	C12C—C13C	1.398 (5)
C14A—C15A	1.513 (5)	C12C—C14C	1.516 (4)
C14A—C45A	1.546 (5)	C13C—H13C	0.9500
C14A—H14A	1.0000	C14C—C15C	1.514 (5)
C15A—C20A	1.397 (5)	C14C—C45C	1.535 (5)
C15A—C16A	1.400 (4)	C14C—H14C	1.0000
C16A—C17A	1.393 (5)	C15C—C16C	1.396 (5)
C17A—C18A	1.387 (5)	C15C—C20C	1.397 (5)
C17A—H17A	0.9500	C16C—C17C	1.381 (5)
C18A—C19A	1.405 (4)	C17C—C18C	1.393 (5)
C19A—C20A	1.384 (5)	C17C—H17C	0.9500
C19A—C21A	1.518 (5)	C18C—O10C	1.387 (5)
C20A—H20A	0.9500	C18C—C19C	1.395 (5)
C21A—C57A	1.531 (5)	C19C—C20C	1.388 (5)
C21A—C22A	1.534 (5)	C19C—C21C	1.519 (5)
C21A—H21A	1.0000	C20C—H20C	0.9500
C22A—C27A	1.393 (4)	C21C—C22C	1.519 (5)
C22A—C23A	1.397 (5)	C21C—C57C	1.528 (5)
C23A—C24A	1.395 (5)	C21C—H21C	1.0000
C24A—C25A	1.383 (5)	C22C—C27C	1.394 (5)
C24A—H24A	0.9500	C22C—C23C	1.402 (5)
C25A—C26A	1.398 (5)	C23C—C24C	1.397 (5)
C26A—C27A	1.395 (5)	C24C—C25C	1.384 (5)
C26A—C28A	1.522 (4)	C24C—H24C	0.9500
C27A—H27A	0.9500	C25C—C26C	1.397 (5)
C28A—C69A	1.543 (5)	C26C—C27C	1.401 (5)
C28A—H28A	1.0000	C26C—C28C	1.517 (4)
C29A—H29A	0.9800	C27C—H27C	0.9500
C29A—H29B	0.9800	C28C—C69C	1.548 (5)
C29A—H29C	0.9800	C28C—H28C	1.0000
C30A—C31A	1.500 (6)	C29C—H29G	0.9800
C30A—H30A	0.9900	C29C—H29H	0.9800

C30A—H30B	0.9900	C29C—H29I	0.9800
C32A—H32A	0.9800	C30C—C31C	1.521 (6)
C32A—H32B	0.9800	C30C—H30E	0.9900
C32A—H32C	0.9800	C30C—H30F	0.9900
C33A—C34A	1.535 (5)	C32C—H32G	0.9800
C33A—H33A	0.9900	C32C—H32H	0.9800
C33A—H33B	0.9900	C32C—H32I	0.9800
C34A—C35A	1.508 (5)	C33C—C34C	1.537 (5)
C34A—H34A	0.9900	C33C—H33E	0.9900
C34A—H34B	0.9900	C33C—H33F	0.9900
C35A—C40A	1.387 (5)	C34C—C35C	1.521 (5)
C35A—C36A	1.397 (5)	C34C—H34E	0.9900
C36A—C37A	1.378 (6)	C34C—H34F	0.9900
C36A—H36A	0.9500	C35C—C40C	1.370 (5)
C37A—C38A	1.380 (6)	C35C—C36C	1.387 (6)
C37A—H37A	0.9500	C36C—C37C	1.389 (7)
C38A—C39A	1.370 (6)	C36C—H36C	0.9500
C38A—H38A	0.9500	C37C—C38C	1.360 (7)
C39A—C40A	1.391 (6)	C37C—H37C	0.9500
C39A—H39A	0.9500	C38C—C39C	1.373 (7)
C40A—H40A	0.9500	C38C—H38C	0.9500
C41A—H41A	0.9800	C39C—C40C	1.395 (6)
C41A—H41B	0.9800	C39C—H39C	0.9500
C41A—H41C	0.9800	C40C—H40C	0.9500
C42A—C43A	1.513 (5)	C41C—H41G	0.9800
C42A—H42A	0.9900	C41C—H41H	0.9800
C42A—H42B	0.9900	C41C—H41I	0.9800
C44A—H44A	0.9800	C42C—C43C	1.508 (6)
C44A—H44B	0.9800	C42C—H42E	0.9900
C44A—H44C	0.9800	C42C—H42F	0.9900
C45A—C46A	1.534 (5)	C44C—H44G	0.9800
C45A—H45A	0.9900	C44C—H44H	0.9800
C45A—H45B	0.9900	C44C—H44I	0.9800
C46A—C47A	1.500 (6)	C45C—C46C	1.524 (5)
C46A—H46A	0.9900	C45C—H45E	0.9900
C46A—H46B	0.9900	C45C—H45F	0.9900
C47A—C48A	1.390 (7)	C46C—C47C	1.521 (6)
C47A—C52A	1.393 (7)	C46C—H46E	0.9900
C48A—C49A	1.388 (7)	C46C—H46F	0.9900
C48A—H48A	0.9500	C47C—C52C	1.374 (7)
C49A—C50A	1.365 (8)	C47C—C48C	1.381 (7)
C49A—H49A	0.9500	C48C—C49C	1.377 (7)
C50A—C51A	1.372 (8)	C48C—H48C	0.9500
C50A—H50A	0.9500	C49C—C50C	1.377 (8)
C51A—C52A	1.372 (7)	C49C—H49C	0.9500
C51A—H51A	0.9500	C50C—C51C	1.357 (8)
C52A—H52A	0.9500	C50C—H50C	0.9500
C53A—H53A	0.9800	C51C—C52C	1.390 (7)
C53A—H53B	0.9800	C51C—H51C	0.9500

supplementary materials

C53A—H53C	0.9800	C52C—H52C	0.9500
C54A—C55A	1.503 (6)	C53C—H53G	0.9800
C54A—H54A	0.9900	C53C—H53H	0.9800
C54A—H54B	0.9900	C53C—H53I	0.9800
C56A—H56A	0.9800	C56C—H56G	0.9800
C56A—H56B	0.9800	C56C—H56H	0.9800
C56A—H56C	0.9800	C56C—H56I	0.9800
C57A—C58A	1.532 (5)	C57C—C58C	1.527 (5)
C57A—H57A	0.9900	C57C—H57E	0.9900
C57A—H57B	0.9900	C57C—H57F	0.9900
C58A—C59A	1.496 (6)	C58C—C59C	1.508 (6)
C58A—H58A	0.9900	C58C—H58E	0.9900
C58A—H58B	0.9900	C58C—H58F	0.9900
C59A—C60A	1.373 (7)	C59C—C60C	1.368 (7)
C59A—C64A	1.398 (6)	C59C—C64C	1.392 (6)
C60A—C61A	1.406 (6)	C60C—C61C	1.387 (7)
C60A—H60A	0.9500	C60C—H60C	0.9500
C61A—C62A	1.354 (8)	C61C—C62C	1.370 (9)
C61A—H61A	0.9500	C61C—H61C	0.9500
C62A—C63A	1.360 (9)	C62C—C63C	1.373 (10)
C62A—H62A	0.9500	C62C—H62C	0.9500
C63A—C64A	1.397 (8)	C63C—C64C	1.371 (9)
C63A—H63A	0.9500	C63C—H63C	0.9500
C64A—H64A	0.9500	C64C—H64C	0.9500
C65A—H65A	0.9800	C65C—H65G	0.9800
C65A—H65B	0.9800	C65C—H65H	0.9800
C65A—H65C	0.9800	C65C—H65I	0.9800
C66A—C67A	1.513 (6)	C66C—C67C	1.485 (6)
C66A—H66A	0.9900	C66C—H66E	0.9900
C66A—H66B	0.9900	C66C—H66F	0.9900
C68A—H68A	0.9800	C68C—H68G	0.9800
C68A—H68B	0.9800	C68C—H68H	0.9800
C68A—H68C	0.9800	C68C—H68I	0.9800
C69A—C70A	1.542 (5)	C69C—C70C	1.539 (5)
C69A—H69A	0.9900	C69C—H69E	0.9900
C69A—H69B	0.9900	C69C—H69F	0.9900
C70A—C71A	1.509 (5)	C70C—C71C	1.498 (6)
C70A—H70A	0.9900	C70C—H70E	0.9900
C70A—H70B	0.9900	C70C—H70F	0.9900
C71A—C76A	1.376 (6)	C71C—C72C	1.384 (7)
C71A—C72A	1.405 (6)	C71C—C76C	1.391 (7)
C72A—C73A	1.388 (6)	C72C—C73C	1.380 (8)
C72A—H72A	0.9500	C72C—H72C	0.9500
C73A—C74A	1.379 (7)	C73C—C74C	1.384 (13)
C73A—H73A	0.9500	C73C—H73C	0.9500
C74A—C75A	1.374 (8)	C74C—C75C	1.394 (13)
C74A—H74A	0.9500	C74C—H74C	0.9500
C75A—C76A	1.407 (7)	C75C—C76C	1.394 (9)
C75A—H75A	0.9500	C75C—H75C	0.9500

C76A—H76A	0.9500	C76C—H76C	0.9500
O1B—C2B	1.380 (4)	O1D—C2D	1.370 (4)
O1B—C29B	1.425 (4)	O1D—C29D	1.429 (4)
O2B—C4B	1.380 (4)	O2D—C4D	1.394 (4)
O2B—C30B	1.426 (4)	O2D—C30D	1.436 (4)
O3B—C31B	1.202 (5)	O3D—C31D	1.190 (5)
O4B—C31B	1.317 (5)	O4D—C31D	1.334 (6)
O4B—C32B	1.425 (7)	O4D—C32D	1.453 (6)
O5B—C9B	1.360 (4)	O5D—C9D	1.378 (4)
O5B—C41B	1.420 (5)	O5D—C41D	1.421 (5)
O6B—C11B	1.389 (4)	O6D—C11D	1.396 (4)
O6B—C42B	1.433 (5)	O6D—C42D	1.423 (4)
O7B—C43B	1.209 (7)	O7D—C43D	1.203 (5)
O8B—C43B	1.303 (7)	O8D—C43D	1.325 (5)
O8B—C44B	1.461 (6)	O8D—C44D	1.448 (5)
O9B—C16B	1.375 (4)	O9D—C16D	1.372 (5)
O9B—C53B	1.414 (5)	O9D—C53D	1.403 (5)
O10B—C18B	1.397 (4)	O10D—C18D	1.384 (5)
O10B—C54B	1.420 (5)	O10D—C54D	1.409 (5)
O11B—C55B	1.178 (6)	O11D—C55D	1.176 (6)
O12B—C55B	1.346 (7)	O12D—C55D	1.326 (7)
O12B—C56B	1.444 (8)	O12D—C56D	1.466 (6)
O13B—C23B	1.371 (4)	O13D—C23D	1.378 (4)
O13B—C65B	1.415 (5)	O13D—C65D	1.420 (5)
O14B—C25B	1.398 (4)	O14D—C25D	1.378 (4)
O14B—C66B	1.416 (5)	O14D—C66D	1.402 (4)
O15B—C67B	1.190 (5)	O15D—C67D	1.212 (5)
O16B—C67B	1.316 (5)	O16D—C67D	1.304 (5)
O16B—C68B	1.468 (5)	O16D—C68D	1.459 (4)
C1B—C6B	1.386 (5)	C1D—C6D	1.383 (5)
C1B—C2B	1.394 (4)	C1D—C2D	1.416 (4)
C1B—C28B	1.528 (5)	C1D—C28D	1.519 (5)
C2B—C3B	1.392 (5)	C2D—C3D	1.379 (5)
C3B—C4B	1.396 (5)	C3D—C4D	1.393 (5)
C3B—H3B	0.9500	C3D—H3D	0.9500
C4B—C5B	1.401 (4)	C4D—C5D	1.398 (4)
C5B—C6B	1.387 (5)	C5D—C6D	1.395 (5)
C5B—C7B	1.519 (5)	C5D—C7D	1.521 (5)
C6B—H6B	0.9500	C6D—H6D	0.9500
C7B—C8B	1.528 (4)	C7D—C8D	1.530 (4)
C7B—C33B	1.537 (5)	C7D—C33D	1.542 (5)
C7B—H7B	1.0000	C7D—H7D	1.0000
C8B—C13B	1.383 (4)	C8D—C9D	1.393 (5)
C8B—C9B	1.406 (5)	C8D—C13D	1.399 (4)
C9B—C10B	1.385 (5)	C9D—C10D	1.388 (5)
C10B—C11B	1.390 (5)	C10D—C11D	1.387 (5)
C10B—H10B	0.9500	C10D—H10D	0.9500
C11B—C12B	1.391 (5)	C11D—C12D	1.381 (5)
C12B—C13B	1.401 (5)	C12D—C13D	1.394 (4)

supplementary materials

C12B—C14B	1.517 (4)	C12D—C14D	1.533 (4)
C13B—H13B	0.9500	C13D—H13D	0.9500
C14B—C15B	1.527 (5)	C14D—C15D	1.516 (5)
C14B—C45B	1.535 (5)	C14D—C45D	1.533 (5)
C14B—H14B	1.0000	C14D—H14D	1.0000
C15B—C20B	1.381 (5)	C15D—C20D	1.386 (5)
C15B—C16B	1.402 (4)	C15D—C16D	1.404 (5)
C16B—C17B	1.387 (5)	C16D—C17D	1.388 (6)
C17B—C18B	1.394 (5)	C17D—C18D	1.398 (6)
C17B—H17B	0.9500	C17D—H17D	0.9500
C18B—C19B	1.396 (4)	C18D—C19D	1.387 (5)
C19B—C20B	1.398 (5)	C19D—C20D	1.386 (5)
C19B—C21B	1.525 (5)	C19D—C21D	1.530 (5)
C20B—H20B	0.9500	C20D—H20D	0.9500
C21B—C22B	1.521 (4)	C21D—C22D	1.528 (4)
C21B—C57B	1.544 (5)	C21D—C57D	1.546 (5)
C21B—H21B	1.0000	C21D—H21D	1.0000
C22B—C27B	1.396 (4)	C22D—C27D	1.392 (5)
C22B—C23B	1.408 (5)	C22D—C23D	1.394 (5)
C23B—C24B	1.383 (5)	C23D—C24D	1.393 (5)
C24B—C25B	1.383 (5)	C24D—C25D	1.389 (5)
C24B—H24B	0.9500	C24D—H24D	0.9500
C25B—C26B	1.393 (5)	C25D—C26D	1.394 (5)
C26B—C27B	1.391 (4)	C26D—C27D	1.394 (4)
C26B—C28B	1.524 (4)	C26D—C28D	1.530 (4)
C27B—H27B	0.9500	C27D—H27D	0.9500
C28B—C69B	1.527 (5)	C28D—C69D	1.536 (5)
C28B—H28B	1.0000	C28D—H28D	1.0000
C29B—H29D	0.9800	C29D—H29J	0.9800
C29B—H29E	0.9800	C29D—H29K	0.9800
C29B—H29F	0.9800	C29D—H29L	0.9800
C30B—C31B	1.483 (6)	C30D—C31D	1.499 (5)
C30B—H30C	0.9900	C30D—H30G	0.9900
C30B—H30D	0.9900	C30D—H30H	0.9900
C32B—H32D	0.9800	C32D—H32J	0.9800
C32B—H32E	0.9800	C32D—H32K	0.9800
C32B—H32F	0.9800	C32D—H32L	0.9800
C33B—C34B	1.539 (5)	C33D—C34D	1.535 (5)
C33B—H33C	0.9900	C33D—H33G	0.9900
C33B—H33D	0.9900	C33D—H33H	0.9900
C34B—C35B	1.514 (5)	C34D—C35D	1.511 (5)
C34B—H34C	0.9900	C34D—H34G	0.9900
C34B—H34D	0.9900	C34D—H34H	0.9900
C35B—C36B	1.370 (6)	C35D—C40D	1.388 (5)
C35B—C40B	1.387 (6)	C35D—C36D	1.398 (5)
C36B—C37B	1.385 (6)	C36D—C37D	1.402 (6)
C36B—H36B	0.9500	C36D—H36D	0.9500
C37B—C38B	1.377 (6)	C37D—C38D	1.368 (7)
C37B—H37B	0.9500	C37D—H37D	0.9500

C38B—C39B	1.374 (7)	C38D—C39D	1.376 (7)
C38B—H38B	0.9500	C38D—H38D	0.9500
C39B—C40B	1.377 (6)	C39D—C40D	1.395 (6)
C39B—H39B	0.9500	C39D—H39D	0.9500
C40B—H40B	0.9500	C40D—H40D	0.9500
C41B—H41D	0.9800	C41D—H41J	0.9800
C41B—H41E	0.9800	C41D—H41K	0.9800
C41B—H41F	0.9800	C41D—H41L	0.9800
C42B—C43B	1.491 (6)	C42D—C43D	1.511 (5)
C42B—H42C	0.9900	C42D—H42G	0.9900
C42B—H42D	0.9900	C42D—H42H	0.9900
C44B—H44D	0.9800	C44D—H44J	0.9800
C44B—H44E	0.9800	C44D—H44K	0.9800
C44B—H44F	0.9800	C44D—H44L	0.9800
C45B—C46B	1.538 (5)	C45D—C46D	1.531 (5)
C45B—H45C	0.9900	C45D—H45G	0.9900
C45B—H45D	0.9900	C45D—H45H	0.9900
C46B—C47B	1.519 (5)	C46D—C47D	1.509 (6)
C46B—H46C	0.9900	C46D—H46G	0.9900
C46B—H46D	0.9900	C46D—H46H	0.9900
C47B—C52B	1.378 (6)	C47D—C48D	1.376 (7)
C47B—C48B	1.384 (6)	C47D—C52D	1.390 (7)
C48B—C49B	1.387 (7)	C48D—C49D	1.384 (7)
C48B—H48B	0.9500	C48D—H48D	0.9500
C49B—C50B	1.360 (8)	C49D—C50D	1.390 (8)
C49B—H49B	0.9500	C49D—H49D	0.9500
C50B—C51B	1.395 (7)	C50D—C51D	1.360 (8)
C50B—H50B	0.9500	C50D—H50D	0.9500
C51B—C52B	1.390 (7)	C51D—C52D	1.391 (7)
C51B—H51B	0.9500	C51D—H51D	0.9500
C52B—H52B	0.9500	C52D—H52D	0.9500
C53B—H53D	0.9800	C53D—H53J	0.9800
C53B—H53E	0.9800	C53D—H53K	0.9800
C53B—H53F	0.9800	C53D—H53L	0.9800
C54B—C55B	1.520 (6)	C54D—C55D	1.494 (7)
C54B—H54C	0.9900	C54D—H54G	0.9900
C54B—H54D	0.9900	C54D—H54H	0.9900
C56B—H56D	0.9800	C56D—H56J	0.9800
C56B—H56E	0.9800	C56D—H56K	0.9800
C56B—H56F	0.9800	C56D—H56L	0.9800
C57B—C58B	1.536 (5)	C57D—C58D	1.527 (5)
C57B—H57C	0.9900	C57D—H57G	0.9900
C57B—H57D	0.9900	C57D—H57H	0.9900
C58B—C59B	1.507 (5)	C58D—C59D	1.510 (6)
C58B—H58C	0.9900	C58D—H58G	0.9900
C58B—H58D	0.9900	C58D—H58H	0.9900
C59B—C64B	1.386 (5)	C59D—C64D	1.368 (7)
C59B—C60B	1.388 (5)	C59D—C60D	1.369 (7)
C60B—C61B	1.385 (6)	C60D—C61D	1.392 (8)

supplementary materials

C60B—H60B	0.9500	C60D—H60D	0.9500
C61B—C62B	1.379 (6)	C61D—C62D	1.368 (9)
C61B—H61B	0.9500	C61D—H61D	0.9500
C62B—C63B	1.363 (6)	C62D—C63D	1.348 (9)
C62B—H62B	0.9500	C62D—H62D	0.9500
C63B—C64B	1.390 (6)	C63D—C64D	1.399 (8)
C63B—H63B	0.9500	C63D—H63D	0.9500
C64B—H64B	0.9500	C64D—H64D	0.9500
C65B—H65D	0.9800	C65D—H65J	0.9800
C65B—H65E	0.9800	C65D—H65K	0.9800
C65B—H65F	0.9800	C65D—H65L	0.9800
C66B—C67B	1.527 (5)	C66D—C67D	1.513 (5)
C66B—H66C	0.9900	C66D—H66G	0.9900
C66B—H66D	0.9900	C66D—H66H	0.9900
C68B—H68D	0.9800	C68D—H68J	0.9800
C68B—H68E	0.9800	C68D—H68K	0.9800
C68B—H68F	0.9800	C68D—H68L	0.9800
C69B—C70B	1.532 (5)	C69D—C70D	1.533 (5)
C69B—H69C	0.9900	C69D—H69G	0.9900
C69B—H69D	0.9900	C69D—H69H	0.9900
C70B—C71B	1.507 (6)	C70D—C71D	1.507 (6)
C70B—H70C	0.9900	C70D—H70G	0.9900
C70B—H70D	0.9900	C70D—H70H	0.9900
C71B—C76B	1.363 (7)	C71D—C72D	1.379 (7)
C71B—C72B	1.392 (7)	C71D—C76D	1.392 (8)
C72B—C73B	1.385 (7)	C72D—C73D	1.431 (11)
C72B—H72B	0.9500	C72D—H72D	0.9500
C73B—C74B	1.351 (9)	C73D—C74D	1.389 (13)
C73B—H73B	0.9500	C73D—H73D	0.9500
C74B—C75B	1.355 (9)	C74D—C75D	1.369 (13)
C74B—H74B	0.9500	C74D—H74D	0.9500
C75B—C76B	1.413 (8)	C75D—C76D	1.377 (8)
C75B—H75B	0.9500	C75D—H75D	0.9500
C76B—H76B	0.9500	C76D—H76D	0.9500
C29A—O1A—C2A—C3A	9.2 (6)	C29C—O1C—C2C—C3C	5.1 (6)
C29A—O1A—C2A—C1A	-169.7 (4)	C29C—O1C—C2C—C1C	-175.9 (4)
C6A—C1A—C2A—O1A	175.3 (3)	C6C—C1C—C2C—C3C	0.8 (5)
C28A—C1A—C2A—O1A	-1.1 (5)	C28C—C1C—C2C—C3C	176.5 (3)
C6A—C1A—C2A—C3A	-3.6 (5)	C6C—C1C—C2C—O1C	-178.3 (3)
C28A—C1A—C2A—C3A	-180.0 (3)	C28C—C1C—C2C—O1C	-2.5 (5)
O1A—C2A—C3A—C4A	-175.6 (3)	O1C—C2C—C3C—C4C	178.2 (3)
C1A—C2A—C3A—C4A	3.3 (5)	C1C—C2C—C3C—C4C	-0.8 (6)
C2A—C3A—C4A—C5A	-0.1 (5)	C2C—C3C—C4C—O2C	-178.0 (3)
C2A—C3A—C4A—O2A	176.5 (3)	C2C—C3C—C4C—C5C	0.4 (6)
C30A—O2A—C4A—C3A	102.1 (4)	C30C—O2C—C4C—C3C	-97.2 (4)
C30A—O2A—C4A—C5A	-81.3 (4)	C30C—O2C—C4C—C5C	84.4 (4)
C3A—C4A—C5A—C6A	-2.5 (5)	C3C—C4C—C5C—C6C	0.0 (5)
O2A—C4A—C5A—C6A	-179.0 (3)	O2C—C4C—C5C—C6C	178.4 (3)
C3A—C4A—C5A—C7A	171.2 (3)	C3C—C4C—C5C—C7C	-176.3 (3)

O2A—C4A—C5A—C7A	-5.3 (5)	O2C—C4C—C5C—C7C	2.0 (5)
C4A—C5A—C6A—C1A	2.1 (5)	C4C—C5C—C6C—C1C	0.0 (5)
C7A—C5A—C6A—C1A	-171.7 (3)	C7C—C5C—C6C—C1C	176.3 (3)
C2A—C1A—C6A—C5A	0.9 (5)	C2C—C1C—C6C—C5C	-0.3 (5)
C28A—C1A—C6A—C5A	177.3 (3)	C28C—C1C—C6C—C5C	-176.1 (3)
C6A—C5A—C7A—C8A	-43.1 (4)	C6C—C5C—C7C—C8C	41.1 (4)
C4A—C5A—C7A—C8A	143.5 (3)	C4C—C5C—C7C—C8C	-142.7 (3)
C6A—C5A—C7A—C33A	81.1 (4)	C6C—C5C—C7C—C33C	-85.9 (4)
C4A—C5A—C7A—C33A	-92.3 (4)	C4C—C5C—C7C—C33C	90.3 (4)
C5A—C7A—C8A—C13A	109.5 (4)	C33C—C7C—C8C—C13C	10.2 (5)
C33A—C7A—C8A—C13A	-10.8 (5)	C5C—C7C—C8C—C13C	-113.0 (3)
C5A—C7A—C8A—C9A	-71.8 (4)	C33C—C7C—C8C—C9C	-170.7 (3)
C33A—C7A—C8A—C9A	168.0 (3)	C5C—C7C—C8C—C9C	66.1 (4)
C41A—O5A—C9A—C10A	-3.7 (5)	C41C—O5C—C9C—C10C	3.2 (5)
C41A—O5A—C9A—C8A	177.4 (3)	C41C—O5C—C9C—C8C	-177.7 (3)
C13A—C8A—C9A—O5A	-178.5 (3)	C13C—C8C—C9C—O5C	178.8 (3)
C7A—C8A—C9A—O5A	2.7 (5)	C7C—C8C—C9C—O5C	-0.4 (5)
C13A—C8A—C9A—C10A	2.6 (5)	C13C—C8C—C9C—C10C	-2.1 (5)
C7A—C8A—C9A—C10A	-176.3 (3)	C7C—C8C—C9C—C10C	178.7 (3)
O5A—C9A—C10A—C11A	-178.7 (3)	O5C—C9C—C10C—C11C	179.2 (3)
C8A—C9A—C10A—C11A	0.2 (5)	C8C—C9C—C10C—C11C	0.2 (5)
C9A—C10A—C11A—C12A	-3.0 (5)	C42C—O6C—C11C—C10C	-67.8 (4)
C9A—C10A—C11A—O6A	172.7 (3)	C42C—O6C—C11C—C12C	116.2 (3)
C42A—O6A—C11A—C10A	73.0 (4)	C9C—C10C—C11C—O6C	-174.4 (3)
C42A—O6A—C11A—C12A	-111.2 (4)	C9C—C10C—C11C—C12C	1.4 (5)
C10A—C11A—C12A—C13A	2.7 (5)	O6C—C11C—C12C—C13C	175.0 (3)
O6A—C11A—C12A—C13A	-173.0 (3)	C10C—C11C—C12C—C13C	-1.0 (5)
C10A—C11A—C12A—C14A	-177.8 (3)	O6C—C11C—C12C—C14C	-5.7 (5)
O6A—C11A—C12A—C14A	6.5 (5)	C10C—C11C—C12C—C14C	178.3 (3)
C9A—C8A—C13A—C12A	-2.8 (5)	C9C—C8C—C13C—C12C	2.6 (5)
C7A—C8A—C13A—C12A	176.0 (3)	C7C—C8C—C13C—C12C	-178.3 (3)
C11A—C12A—C13A—C8A	0.2 (5)	C11C—C12C—C13C—C8C	-1.1 (5)
C14A—C12A—C13A—C8A	-179.2 (3)	C14C—C12C—C13C—C8C	179.7 (3)
C11A—C12A—C14A—C15A	69.7 (4)	C11C—C12C—C14C—C15C	-63.2 (4)
C13A—C12A—C14A—C15A	-110.9 (4)	C13C—C12C—C14C—C15C	116.1 (3)
C11A—C12A—C14A—C45A	-165.1 (3)	C11C—C12C—C14C—C45C	170.9 (3)
C13A—C12A—C14A—C45A	14.4 (5)	C13C—C12C—C14C—C45C	-9.8 (5)
C12A—C14A—C15A—C20A	50.4 (4)	C12C—C14C—C15C—C16C	129.2 (3)
C45A—C14A—C15A—C20A	-76.4 (4)	C45C—C14C—C15C—C16C	-103.6 (4)
C12A—C14A—C15A—C16A	-129.9 (3)	C12C—C14C—C15C—C20C	-46.6 (4)
C45A—C14A—C15A—C16A	103.3 (4)	C45C—C14C—C15C—C20C	80.5 (4)
C53A—O9A—C16A—C17A	9.7 (6)	C53C—O9C—C16C—C17C	-3.7 (6)
C53A—O9A—C16A—C15A	-171.4 (4)	C53C—O9C—C16C—C15C	176.8 (4)
C20A—C15A—C16A—O9A	-176.7 (3)	C20C—C15C—C16C—O9C	-178.9 (3)
C14A—C15A—C16A—O9A	3.6 (5)	C14C—C15C—C16C—O9C	5.1 (5)
C20A—C15A—C16A—C17A	2.3 (5)	C20C—C15C—C16C—C17C	1.7 (5)
C14A—C15A—C16A—C17A	-177.4 (3)	C14C—C15C—C16C—C17C	-174.3 (3)
O9A—C16A—C17A—C18A	178.3 (3)	O9C—C16C—C17C—C18C	-178.9 (4)
C15A—C16A—C17A—C18A	-0.5 (5)	C15C—C16C—C17C—C18C	0.5 (6)

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C54A—O10A—C18A—C17A	1.5 (5)	C16C—C17C—C18C—O10C	178.1 (4)
C54A—O10A—C18A—C19A	-179.7 (3)	C16C—C17C—C18C—C19C	-3.6 (6)
C16A—C17A—C18A—O10A	176.7 (3)	O10C—C18C—C19C—C20C	-177.4 (3)
C16A—C17A—C18A—C19A	-1.9 (5)	C17C—C18C—C19C—C20C	4.2 (5)
O10A—C18A—C19A—C20A	-176.3 (3)	O10C—C18C—C19C—C21C	2.1 (5)
C17A—C18A—C19A—C20A	2.4 (5)	C17C—C18C—C19C—C21C	-176.4 (4)
O10A—C18A—C19A—C21A	4.7 (5)	C18C—C19C—C20C—C15C	-1.9 (5)
C17A—C18A—C19A—C21A	-176.5 (3)	C21C—C19C—C20C—C15C	178.6 (3)
C18A—C19A—C20A—C15A	-0.6 (5)	C16C—C15C—C20C—C19C	-1.0 (5)
C21A—C19A—C20A—C15A	178.4 (3)	C14C—C15C—C20C—C19C	175.1 (3)
C16A—C15A—C20A—C19A	-1.7 (5)	C20C—C19C—C21C—C22C	50.3 (5)
C14A—C15A—C20A—C19A	178.0 (3)	C18C—C19C—C21C—C22C	-129.2 (4)
C20A—C19A—C21A—C57A	83.0 (4)	C20C—C19C—C21C—C57C	-76.0 (4)
C18A—C19A—C21A—C57A	-98.1 (4)	C18C—C19C—C21C—C57C	104.6 (4)
C20A—C19A—C21A—C22A	-42.7 (4)	C19C—C21C—C22C—C27C	-111.7 (4)
C18A—C19A—C21A—C22A	136.2 (3)	C57C—C21C—C22C—C27C	13.3 (5)
C19A—C21A—C22A—C27A	113.5 (4)	C19C—C21C—C22C—C23C	69.6 (4)
C57A—C21A—C22A—C27A	-11.2 (5)	C57C—C21C—C22C—C23C	-165.4 (3)
C19A—C21A—C22A—C23A	-67.6 (4)	C65C—O13C—C23C—C24C	6.8 (5)
C57A—C21A—C22A—C23A	167.6 (3)	C65C—O13C—C23C—C22C	-173.6 (4)
C65A—O13A—C23A—C24A	-12.6 (5)	C27C—C22C—C23C—O13C	179.8 (3)
C65A—O13A—C23A—C22A	168.3 (3)	C21C—C22C—C23C—O13C	-1.4 (5)
C27A—C22A—C23A—O13A	178.9 (3)	C27C—C22C—C23C—C24C	-0.7 (5)
C21A—C22A—C23A—O13A	0.0 (5)	C21C—C22C—C23C—C24C	178.1 (3)
C27A—C22A—C23A—C24A	-0.1 (5)	O13C—C23C—C24C—C25C	179.8 (3)
C21A—C22A—C23A—C24A	-179.0 (3)	C22C—C23C—C24C—C25C	0.3 (5)
O13A—C23A—C24A—C25A	-178.0 (3)	C23C—C24C—C25C—C26C	0.2 (6)
C22A—C23A—C24A—C25A	1.0 (5)	C23C—C24C—C25C—O14C	-177.4 (3)
C66A—O14A—C25A—C24A	45.0 (5)	C66C—O14C—C25C—C24C	-58.6 (6)
C66A—O14A—C25A—C26A	-136.0 (4)	C66C—O14C—C25C—C26C	123.6 (5)
C23A—C24A—C25A—O14A	178.4 (3)	C24C—C25C—C26C—C27C	-0.3 (5)
C23A—C24A—C25A—C26A	-0.6 (5)	O14C—C25C—C26C—C27C	177.5 (3)
O14A—C25A—C26A—C27A	-179.7 (3)	C24C—C25C—C26C—C28C	177.9 (3)
C24A—C25A—C26A—C27A	-0.7 (5)	O14C—C25C—C26C—C28C	-4.4 (5)
O14A—C25A—C26A—C28A	3.2 (5)	C23C—C22C—C27C—C26C	0.6 (5)
C24A—C25A—C26A—C28A	-177.8 (3)	C21C—C22C—C27C—C26C	-178.2 (3)
C23A—C22A—C27A—C26A	-1.2 (5)	C25C—C26C—C27C—C22C	-0.1 (5)
C21A—C22A—C27A—C26A	177.7 (3)	C28C—C26C—C27C—C22C	-178.3 (3)
C25A—C26A—C27A—C22A	1.6 (5)	C6C—C1C—C28C—C26C	-46.2 (4)
C28A—C26A—C27A—C22A	178.6 (3)	C2C—C1C—C28C—C26C	138.2 (3)
C27A—C26A—C28A—C1A	-116.2 (4)	C6C—C1C—C28C—C69C	80.0 (4)
C25A—C26A—C28A—C1A	60.7 (4)	C2C—C1C—C28C—C69C	-95.6 (4)
C27A—C26A—C28A—C69A	7.2 (5)	C25C—C26C—C28C—C1C	-65.1 (4)
C25A—C26A—C28A—C69A	-176.0 (3)	C27C—C26C—C28C—C1C	113.0 (4)
C6A—C1A—C28A—C26A	41.3 (4)	C25C—C26C—C28C—C69C	173.0 (3)
C2A—C1A—C28A—C26A	-142.4 (3)	C27C—C26C—C28C—C69C	-8.9 (5)
C6A—C1A—C28A—C69A	-85.6 (4)	C4C—O2C—C30C—C31C	80.6 (4)
C2A—C1A—C28A—C69A	90.6 (4)	C32C—O4C—C31C—O3C	-0.3 (8)
C4A—O2A—C30A—C31A	-88.5 (4)	C32C—O4C—C31C—C30C	-178.8 (5)

C32A—O4A—C31A—O3A	2.8 (8)	O2C—C30C—C31C—O3C	23.6 (7)
C32A—O4A—C31A—C30A	-178.2 (5)	O2C—C30C—C31C—O4C	-158.0 (3)
O2A—C30A—C31A—O3A	-7.1 (7)	C8C—C7C—C33C—C34C	68.0 (4)
O2A—C30A—C31A—O4A	173.9 (3)	C5C—C7C—C33C—C34C	-167.3 (3)
C5A—C7A—C33A—C34A	168.7 (3)	C7C—C33C—C34C—C35C	-177.3 (3)
C8A—C7A—C33A—C34A	-67.9 (4)	C33C—C34C—C35C—C40C	89.3 (4)
C7A—C33A—C34A—C35A	174.2 (3)	C33C—C34C—C35C—C36C	-88.2 (5)
C33A—C34A—C35A—C40A	-97.4 (4)	C40C—C35C—C36C—C37C	0.0 (7)
C33A—C34A—C35A—C36A	80.2 (4)	C34C—C35C—C36C—C37C	177.5 (4)
C40A—C35A—C36A—C37A	0.8 (6)	C35C—C36C—C37C—C38C	0.4 (8)
C34A—C35A—C36A—C37A	-177.0 (4)	C36C—C37C—C38C—C39C	0.1 (8)
C35A—C36A—C37A—C38A	-0.9 (7)	C37C—C38C—C39C—C40C	-1.0 (8)
C36A—C37A—C38A—C39A	0.8 (7)	C36C—C35C—C40C—C39C	-0.8 (7)
C37A—C38A—C39A—C40A	-0.6 (7)	C34C—C35C—C40C—C39C	-178.4 (4)
C36A—C35A—C40A—C39A	-0.6 (6)	C38C—C39C—C40C—C35C	1.3 (7)
C34A—C35A—C40A—C39A	177.1 (4)	C11C—O6C—C42C—C43C	-176.8 (3)
C38A—C39A—C40A—C35A	0.5 (7)	C44C—O8C—C43C—O7C	1.3 (7)
C11A—O6A—C42A—C43A	173.9 (3)	C44C—O8C—C43C—C42C	-176.6 (4)
C44A—O8A—C43A—O7A	1.0 (6)	O6C—C42C—C43C—O7C	154.8 (4)
C44A—O8A—C43A—C42A	178.9 (4)	O6C—C42C—C43C—O8C	-27.2 (5)
O6A—C42A—C43A—O7A	-151.3 (4)	C15C—C14C—C45C—C46C	65.2 (4)
O6A—C42A—C43A—O8A	30.7 (5)	C12C—C14C—C45C—C46C	-170.0 (3)
C12A—C14A—C45A—C46A	170.6 (3)	C14C—C45C—C46C—C47C	170.9 (4)
C15A—C14A—C45A—C46A	-64.1 (4)	C45C—C46C—C47C—C52C	108.4 (4)
C14A—C45A—C46A—C47A	-171.9 (4)	C45C—C46C—C47C—C48C	-72.3 (5)
C45A—C46A—C47A—C48A	-109.1 (4)	C52C—C47C—C48C—C49C	-0.5 (7)
C45A—C46A—C47A—C52A	72.6 (5)	C46C—C47C—C48C—C49C	-179.8 (4)
C52A—C47A—C48A—C49A	0.8 (5)	C47C—C48C—C49C—C50C	2.4 (8)
C46A—C47A—C48A—C49A	-177.6 (4)	C48C—C49C—C50C—C51C	-2.4 (8)
C47A—C48A—C49A—C50A	-1.1 (6)	C49C—C50C—C51C—C52C	0.6 (7)
C48A—C49A—C50A—C51A	0.8 (7)	C48C—C47C—C52C—C51C	-1.4 (6)
C49A—C50A—C51A—C52A	-0.2 (8)	C46C—C47C—C52C—C51C	177.9 (4)
C50A—C51A—C52A—C47A	-0.2 (8)	C50C—C51C—C52C—C47C	1.3 (6)
C48A—C47A—C52A—C51A	-0.1 (7)	C17C—C18C—O10C—C54C	-30.1 (6)
C46A—C47A—C52A—C51A	178.3 (4)	C19C—C18C—O10C—C54C	151.5 (4)
C18A—O10A—C54A—C55A	75.9 (4)	C55C—C54C—O10C—C18C	93.5 (6)
C56A—O12A—C55A—O11A	-0.9 (8)	C56C—O12C—C55C—O11C	0.4 (11)
C56A—O12A—C55A—C54A	175.6 (4)	C56C—O12C—C55C—C54C	-178.4 (6)
O10A—C54A—C55A—O11A	40.8 (7)	O10C—C54C—C55C—O11C	175.9 (7)
O10A—C54A—C55A—O12A	-135.7 (4)	O10C—C54C—C55C—O12C	-5.3 (8)
C19A—C21A—C57A—C58A	63.9 (4)	C19C—C21C—C57C—C58C	-60.4 (4)
C22A—C21A—C57A—C58A	-171.7 (3)	C22C—C21C—C57C—C58C	173.5 (3)
C21A—C57A—C58A—C59A	179.7 (4)	C21C—C57C—C58C—C59C	173.4 (3)
C57A—C58A—C59A—C60A	103.6 (4)	C57C—C58C—C59C—C60C	38.3 (6)
C57A—C58A—C59A—C64A	-73.5 (5)	C57C—C58C—C59C—C64C	-140.5 (4)
C64A—C59A—C60A—C61A	0.4 (6)	C64C—C59C—C60C—C61C	0.2 (8)
C58A—C59A—C60A—C61A	-176.9 (4)	C58C—C59C—C60C—C61C	-178.6 (5)
C59A—C60A—C61A—C62A	-1.5 (7)	C59C—C60C—C61C—C62C	0.3 (9)
C60A—C61A—C62A—C63A	0.8 (8)	C60C—C61C—C62C—C63C	-1.8 (9)

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C61A—C62A—C63A—C64A	0.9 (8)	C61C—C62C—C63C—C64C	2.8 (9)
C62A—C63A—C64A—C59A	-2.0 (7)	C62C—C63C—C64C—C59C	-2.3 (9)
C60A—C59A—C64A—C63A	1.3 (6)	C60C—C59C—C64C—C63C	0.8 (7)
C58A—C59A—C64A—C63A	178.6 (4)	C58C—C59C—C64C—C63C	179.6 (5)
C25A—O14A—C66A—C67A	163.3 (4)	C25C—O14C—C66C—C67C	-174.7 (5)
C68A—O16A—C67A—O15A	-2.2 (8)	C68C—O16C—C67C—O15C	-2.3 (9)
C68A—O16A—C67A—C66A	177.2 (4)	C68C—O16C—C67C—C66C	179.0 (5)
O14A—C66A—C67A—O15A	-165.1 (5)	O14C—C66C—C67C—O15C	178.2 (6)
O14A—C66A—C67A—O16A	15.5 (6)	O14C—C66C—C67C—O16C	-3.1 (8)
C26A—C28A—C69A—C70A	68.2 (4)	C1C—C28C—C69C—C70C	166.4 (3)
C1A—C28A—C69A—C70A	-167.4 (3)	C26C—C28C—C69C—C70C	-69.8 (4)
C28A—C69A—C70A—C71A	-175.5 (3)	C28C—C69C—C70C—C71C	-174.4 (3)
C69A—C70A—C71A—C76A	-90.9 (5)	C69C—C70C—C71C—C72C	-75.2 (5)
C69A—C70A—C71A—C72A	84.1 (4)	C69C—C70C—C71C—C76C	100.0 (5)
C76A—C71A—C72A—C73A	-0.9 (7)	C76C—C71C—C72C—C73C	0.3 (8)
C70A—C71A—C72A—C73A	-176.0 (4)	C70C—C71C—C72C—C73C	175.4 (5)
C71A—C72A—C73A—C74A	0.8 (7)	C71C—C72C—C73C—C74C	-1.6 (10)
C72A—C73A—C74A—C75A	-0.8 (8)	C72C—C73C—C74C—C75C	2.6 (12)
C73A—C74A—C75A—C76A	0.8 (8)	C73C—C74C—C75C—C76C	-2.2 (13)
C72A—C71A—C76A—C75A	0.9 (7)	C72C—C71C—C76C—C75C	0.1 (8)
C70A—C71A—C76A—C75A	176.0 (4)	C70C—C71C—C76C—C75C	-175.1 (5)
C74A—C75A—C76A—C71A	-0.9 (8)	C74C—C75C—C76C—C71C	0.9 (10)
C29B—O1B—C2B—C3B	-8.1 (5)	C29D—O1D—C2D—C3D	-7.2 (5)
C29B—O1B—C2B—C1B	173.4 (4)	C29D—O1D—C2D—C1D	173.6 (3)
C6B—C1B—C2B—O1B	176.2 (3)	C6D—C1D—C2D—O1D	179.4 (3)
C28B—C1B—C2B—O1B	-3.5 (5)	C28D—C1D—C2D—O1D	2.0 (5)
C6B—C1B—C2B—C3B	-2.3 (5)	C6D—C1D—C2D—C3D	0.1 (5)
C28B—C1B—C2B—C3B	178.0 (3)	C28D—C1D—C2D—C3D	-177.2 (3)
O1B—C2B—C3B—C4B	-178.1 (3)	O1D—C2D—C3D—C4D	-178.9 (3)
C1B—C2B—C3B—C4B	0.3 (5)	C1D—C2D—C3D—C4D	0.3 (5)
C30B—O2B—C4B—C3B	-6.1 (5)	C2D—C3D—C4D—O2D	178.4 (3)
C30B—O2B—C4B—C5B	174.1 (3)	C2D—C3D—C4D—C5D	-0.8 (5)
C2B—C3B—C4B—O2B	-177.5 (3)	C30D—O2D—C4D—C3D	95.8 (4)
C2B—C3B—C4B—C5B	2.3 (5)	C30D—O2D—C4D—C5D	-85.0 (4)
O2B—C4B—C5B—C6B	177.0 (3)	C3D—C4D—C5D—C6D	0.9 (5)
C3B—C4B—C5B—C6B	-2.9 (5)	O2D—C4D—C5D—C6D	-178.3 (3)
O2B—C4B—C5B—C7B	-5.2 (5)	C3D—C4D—C5D—C7D	176.4 (3)
C3B—C4B—C5B—C7B	175.0 (3)	O2D—C4D—C5D—C7D	-2.7 (5)
C2B—C1B—C6B—C5B	1.8 (5)	C2D—C1D—C6D—C5D	-0.1 (5)
C28B—C1B—C6B—C5B	-178.5 (3)	C28D—C1D—C6D—C5D	177.3 (3)
C4B—C5B—C6B—C1B	0.8 (5)	C4D—C5D—C6D—C1D	-0.4 (5)
C7B—C5B—C6B—C1B	-177.1 (3)	C7D—C5D—C6D—C1D	-176.0 (3)
C6B—C5B—C7B—C8B	43.9 (4)	C6D—C5D—C7D—C8D	-42.2 (4)
C4B—C5B—C7B—C8B	-133.9 (3)	C4D—C5D—C7D—C8D	142.5 (3)
C6B—C5B—C7B—C33B	-83.0 (4)	C6D—C5D—C7D—C33D	84.7 (4)
C4B—C5B—C7B—C33B	99.2 (4)	C4D—C5D—C7D—C33D	-90.6 (4)
C5B—C7B—C8B—C13B	-111.6 (4)	C5D—C7D—C8D—C9D	-67.1 (4)
C33B—C7B—C8B—C13B	14.9 (4)	C33D—C7D—C8D—C9D	169.0 (3)
C5B—C7B—C8B—C9B	68.6 (4)	C5D—C7D—C8D—C13D	113.6 (3)

C33B—C7B—C8B—C9B	-164.9 (3)	C33D—C7D—C8D—C13D	-10.3 (4)
C41B—O5B—C9B—C10B	9.4 (6)	C41D—O5D—C9D—C10D	-8.7 (5)
C41B—O5B—C9B—C8B	-170.6 (4)	C41D—O5D—C9D—C8D	172.1 (3)
C13B—C8B—C9B—O5B	179.5 (3)	C13D—C8D—C9D—O5D	-178.9 (3)
C7B—C8B—C9B—O5B	-0.7 (5)	C7D—C8D—C9D—O5D	1.8 (4)
C13B—C8B—C9B—C10B	-0.4 (5)	C13D—C8D—C9D—C10D	1.9 (5)
C7B—C8B—C9B—C10B	179.4 (3)	C7D—C8D—C9D—C10D	-177.4 (3)
O5B—C9B—C10B—C11B	179.9 (4)	O5D—C9D—C10D—C11D	-179.3 (3)
C8B—C9B—C10B—C11B	-0.2 (6)	C8D—C9D—C10D—C11D	-0.1 (5)
C42B—O6B—C11B—C10B	-64.0 (5)	C9D—C10D—C11D—C12D	-1.2 (5)
C42B—O6B—C11B—C12B	117.4 (4)	C9D—C10D—C11D—O6D	175.3 (3)
C9B—C10B—C11B—O6B	-178.2 (3)	C42D—O6D—C11D—C12D	-117.5 (3)
C9B—C10B—C11B—C12B	0.3 (6)	C42D—O6D—C11D—C10D	66.0 (4)
O6B—C11B—C12B—C13B	178.8 (3)	C10D—C11D—C12D—C13D	0.6 (5)
C10B—C11B—C12B—C13B	0.3 (5)	O6D—C11D—C12D—C13D	-175.8 (3)
O6B—C11B—C12B—C14B	-1.8 (5)	C10D—C11D—C12D—C14D	-177.5 (3)
C10B—C11B—C12B—C14B	179.6 (3)	O6D—C11D—C12D—C14D	6.0 (5)
C9B—C8B—C13B—C12B	1.1 (5)	C11D—C12D—C13D—C8D	1.2 (5)
C7B—C8B—C13B—C12B	-178.7 (3)	C14D—C12D—C13D—C8D	179.3 (3)
C11B—C12B—C13B—C8B	-1.0 (5)	C9D—C8D—C13D—C12D	-2.4 (5)
C14B—C12B—C13B—C8B	179.7 (3)	C7D—C8D—C13D—C12D	176.9 (3)
C11B—C12B—C14B—C15B	-64.3 (4)	C11D—C12D—C14D—C15D	62.6 (4)
C13B—C12B—C14B—C15B	115.0 (4)	C13D—C12D—C14D—C15D	-115.4 (4)
C11B—C12B—C14B—C45B	173.1 (3)	C11D—C12D—C14D—C45D	-170.4 (3)
C13B—C12B—C14B—C45B	-7.6 (5)	C13D—C12D—C14D—C45D	11.6 (5)
C12B—C14B—C15B—C20B	-41.6 (4)	C45D—C14D—C15D—C20D	-79.5 (4)
C45B—C14B—C15B—C20B	85.3 (4)	C12D—C14D—C15D—C20D	47.5 (4)
C12B—C14B—C15B—C16B	143.4 (3)	C45D—C14D—C15D—C16D	105.2 (4)
C45B—C14B—C15B—C16B	-89.7 (4)	C12D—C14D—C15D—C16D	-127.7 (3)
C53B—O9B—C16B—C17B	-14.0 (7)	C53D—O9D—C16D—C17D	1.4 (6)
C53B—O9B—C16B—C15B	165.5 (5)	C53D—O9D—C16D—C15D	-179.8 (4)
C20B—C15B—C16B—O9B	-176.4 (3)	C20D—C15D—C16D—O9D	178.9 (3)
C14B—C15B—C16B—O9B	-1.3 (5)	C14D—C15D—C16D—O9D	-5.7 (5)
C20B—C15B—C16B—C17B	3.1 (5)	C20D—C15D—C16D—C17D	-2.3 (5)
C14B—C15B—C16B—C17B	178.3 (3)	C14D—C15D—C16D—C17D	173.2 (3)
O9B—C16B—C17B—C18B	177.3 (4)	O9D—C16D—C17D—C18D	178.9 (4)
C15B—C16B—C17B—C18B	-2.2 (6)	C15D—C16D—C17D—C18D	0.1 (6)
C16B—C17B—C18B—C19B	-0.7 (6)	C54D—O10D—C18D—C19D	-151.7 (4)
C16B—C17B—C18B—O10B	-176.4 (3)	C54D—O10D—C18D—C17D	28.7 (6)
C54B—O10B—C18B—C17B	-102.2 (4)	C16D—C17D—C18D—O10D	-178.0 (4)
C54B—O10B—C18B—C19B	82.0 (4)	C16D—C17D—C18D—C19D	2.3 (6)
C17B—C18B—C19B—C20B	2.5 (5)	O10D—C18D—C19D—C20D	178.0 (3)
O10B—C18B—C19B—C20B	178.2 (3)	C17D—C18D—C19D—C20D	-2.4 (5)
C17B—C18B—C19B—C21B	-171.3 (3)	O10D—C18D—C19D—C21D	-3.3 (5)
O10B—C18B—C19B—C21B	4.4 (5)	C17D—C18D—C19D—C21D	176.4 (3)
C16B—C15B—C20B—C19B	-1.2 (5)	C18D—C19D—C20D—C15D	0.0 (5)
C14B—C15B—C20B—C19B	-176.4 (3)	C21D—C19D—C20D—C15D	-178.7 (3)
C18B—C19B—C20B—C15B	-1.5 (5)	C16D—C15D—C20D—C19D	2.2 (5)
C21B—C19B—C20B—C15B	172.4 (3)	C14D—C15D—C20D—C19D	-173.2 (3)

supplementary materials

C18B—C19B—C21B—C22B	-142.4 (3)	C20D—C19D—C21D—C22D	-50.8 (4)
C20B—C19B—C21B—C22B	44.1 (4)	C18D—C19D—C21D—C22D	130.5 (3)
C18B—C19B—C21B—C57B	91.3 (4)	C20D—C19D—C21D—C57D	75.9 (4)
C20B—C19B—C21B—C57B	-82.2 (4)	C18D—C19D—C21D—C57D	-102.8 (4)
C19B—C21B—C22B—C27B	-110.1 (3)	C19D—C21D—C22D—C27D	114.1 (4)
C57B—C21B—C22B—C27B	12.5 (4)	C57D—C21D—C22D—C27D	-11.0 (5)
C19B—C21B—C22B—C23B	70.0 (4)	C19D—C21D—C22D—C23D	-66.7 (4)
C57B—C21B—C22B—C23B	-167.4 (3)	C57D—C21D—C22D—C23D	168.3 (3)
C65B—O13B—C23B—C24B	2.9 (5)	C65D—O13D—C23D—C24D	-9.9 (5)
C65B—O13B—C23B—C22B	-179.4 (3)	C65D—O13D—C23D—C22D	171.0 (3)
C27B—C22B—C23B—O13B	178.4 (3)	C27D—C22D—C23D—O13D	-177.7 (3)
C21B—C22B—C23B—O13B	-1.7 (5)	C21D—C22D—C23D—O13D	2.9 (5)
C27B—C22B—C23B—C24B	-3.8 (5)	C27D—C22D—C23D—C24D	3.2 (5)
C21B—C22B—C23B—C24B	176.1 (3)	C21D—C22D—C23D—C24D	-176.1 (3)
O13B—C23B—C24B—C25B	179.2 (3)	O13D—C23D—C24D—C25D	179.9 (3)
C22B—C23B—C24B—C25B	1.6 (5)	C22D—C23D—C24D—C25D	-1.1 (5)
C23B—C24B—C25B—C26B	1.2 (5)	C66D—O14D—C25D—C24D	15.7 (5)
C23B—C24B—C25B—O14B	-172.0 (3)	C66D—O14D—C25D—C26D	-163.0 (3)
C66B—O14B—C25B—C24B	-75.8 (4)	C23D—C24D—C25D—O14D	179.2 (3)
C66B—O14B—C25B—C26B	110.8 (4)	C23D—C24D—C25D—C26D	-2.2 (5)
C24B—C25B—C26B—C27B	-1.5 (5)	O14D—C25D—C26D—C27D	-178.3 (3)
O14B—C25B—C26B—C27B	171.9 (3)	C24D—C25D—C26D—C27D	3.1 (5)
C24B—C25B—C26B—C28B	179.0 (3)	O14D—C25D—C26D—C28D	4.3 (5)
O14B—C25B—C26B—C28B	-7.7 (5)	C24D—C25D—C26D—C28D	-174.3 (3)
C25B—C26B—C27B—C22B	-1.0 (5)	C23D—C22D—C27D—C26D	-2.3 (5)
C28B—C26B—C27B—C22B	178.5 (3)	C21D—C22D—C27D—C26D	177.0 (3)
C23B—C22B—C27B—C26B	3.6 (5)	C25D—C26D—C27D—C22D	-0.8 (5)
C21B—C22B—C27B—C26B	-176.3 (3)	C28D—C26D—C27D—C22D	176.5 (3)
C27B—C26B—C28B—C69B	-16.6 (5)	C6D—C1D—C28D—C26D	46.8 (4)
C25B—C26B—C28B—C69B	162.9 (3)	C2D—C1D—C28D—C26D	-136.0 (3)
C27B—C26B—C28B—C1B	109.8 (4)	C6D—C1D—C28D—C69D	-78.9 (4)
C25B—C26B—C28B—C1B	-70.7 (4)	C2D—C1D—C28D—C69D	98.3 (4)
C6B—C1B—C28B—C26B	-50.6 (4)	C27D—C26D—C28D—C1D	-114.1 (4)
C2B—C1B—C28B—C26B	129.1 (3)	C25D—C26D—C28D—C1D	63.1 (4)
C6B—C1B—C28B—C69B	77.5 (4)	C27D—C26D—C28D—C69D	7.2 (5)
C2B—C1B—C28B—C69B	-102.8 (4)	C25D—C26D—C28D—C69D	-175.6 (3)
C4B—O2B—C30B—C31B	-69.8 (4)	C4D—O2D—C30D—C31D	-80.3 (4)
C32B—O4B—C31B—O3B	2.3 (8)	C32D—O4D—C31D—O3D	1.5 (7)
C32B—O4B—C31B—C30B	-177.1 (5)	C32D—O4D—C31D—C30D	178.8 (4)
O2B—C30B—C31B—O3B	-22.0 (6)	O2D—C30D—C31D—O3D	-28.2 (6)
O2B—C30B—C31B—O4B	157.4 (4)	O2D—C30D—C31D—O4D	154.6 (3)
C5B—C7B—C33B—C34B	-63.3 (4)	C5D—C7D—C33D—C34D	166.2 (3)
C8B—C7B—C33B—C34B	170.8 (3)	C8D—C7D—C33D—C34D	-68.6 (4)
C7B—C33B—C34B—C35B	177.5 (3)	C7D—C33D—C34D—C35D	176.3 (3)
C33B—C34B—C35B—C36B	67.9 (5)	C33D—C34D—C35D—C40D	-91.3 (4)
C33B—C34B—C35B—C40B	-111.1 (4)	C33D—C34D—C35D—C36D	86.7 (4)
C40B—C35B—C36B—C37B	-0.6 (7)	C40D—C35D—C36D—C37D	1.7 (6)
C34B—C35B—C36B—C37B	-179.7 (4)	C34D—C35D—C36D—C37D	-176.3 (4)
C35B—C36B—C37B—C38B	-0.3 (7)	C35D—C36D—C37D—C38D	-1.6 (7)

C36B—C37B—C38B—C39B	1.0 (7)	C36D—C37D—C38D—C39D	0.7 (7)
C37B—C38B—C39B—C40B	-0.8 (7)	C37D—C38D—C39D—C40D	0.2 (7)
C38B—C39B—C40B—C35B	-0.1 (7)	C36D—C35D—C40D—C39D	-0.9 (6)
C36B—C35B—C40B—C39B	0.8 (6)	C34D—C35D—C40D—C39D	177.1 (4)
C34B—C35B—C40B—C39B	179.9 (4)	C38D—C39D—C40D—C35D	0.0 (7)
C11B—O6B—C42B—C43B	-162.5 (4)	C11D—O6D—C42D—C43D	179.3 (3)
C44B—O8B—C43B—O7B	-4.1 (9)	C44D—O8D—C43D—O7D	-0.5 (7)
C44B—O8B—C43B—C42B	176.3 (6)	C44D—O8D—C43D—C42D	175.7 (4)
O6B—C42B—C43B—O7B	171.6 (6)	O6D—C42D—C43D—O7D	-158.3 (4)
O6B—C42B—C43B—O8B	-8.7 (7)	O6D—C42D—C43D—O8D	25.4 (5)
C12B—C14B—C45B—C46B	-68.3 (4)	C15D—C14D—C45D—C46D	-65.7 (4)
C15B—C14B—C45B—C46B	167.5 (3)	C12D—C14D—C45D—C46D	169.8 (3)
C14B—C45B—C46B—C47B	173.1 (3)	C14D—C45D—C46D—C47D	-168.0 (4)
C45B—C46B—C47B—C52B	-74.4 (4)	C45D—C46D—C47D—C48D	71.6 (5)
C45B—C46B—C47B—C48B	106.2 (4)	C45D—C46D—C47D—C52D	-110.0 (4)
C52B—C47B—C48B—C49B	0.9 (7)	C52D—C47D—C48D—C49D	-1.5 (6)
C46B—C47B—C48B—C49B	-179.7 (4)	C46D—C47D—C48D—C49D	177.1 (4)
C47B—C48B—C49B—C50B	-0.6 (8)	C47D—C48D—C49D—C50D	0.9 (8)
C48B—C49B—C50B—C51B	0.6 (8)	C48D—C49D—C50D—C51D	-0.9 (7)
C49B—C50B—C51B—C52B	-0.9 (8)	C49D—C50D—C51D—C52D	1.5 (7)
C48B—C47B—C52B—C51B	-1.2 (7)	C48D—C47D—C52D—C51D	2.1 (6)
C46B—C47B—C52B—C51B	179.4 (4)	C46D—C47D—C52D—C51D	-176.4 (4)
C50B—C51B—C52B—C47B	1.2 (7)	C50D—C51D—C52D—C47D	-2.1 (6)
C18B—O10B—C54B—C55B	88.1 (4)	C18D—O10D—C54D—C55D	-94.1 (5)
C56B—O12B—C55B—O11B	-1.5 (9)	C56D—O12D—C55D—O11D	-3.1 (10)
C56B—O12B—C55B—C54B	178.4 (6)	C56D—O12D—C55D—C54D	-178.8 (6)
O10B—C54B—C55B—O11B	5.8 (7)	O10D—C54D—C55D—O11D	-170.8 (6)
O10B—C54B—C55B—O12B	-174.1 (4)	O10D—C54D—C55D—O12D	4.9 (7)
C22B—C21B—C57B—C58B	66.4 (4)	C22D—C21D—C57D—C58D	-166.4 (4)
C19B—C21B—C57B—C58B	-168.6 (3)	C19D—C21D—C57D—C58D	67.8 (4)
C21B—C57B—C58B—C59B	-173.8 (3)	C21D—C57D—C58D—C59D	-170.4 (4)
C57B—C58B—C59B—C64B	98.8 (4)	C57D—C58D—C59D—C64D	116.8 (5)
C57B—C58B—C59B—C60B	-77.1 (4)	C57D—C58D—C59D—C60D	-63.1 (6)
C64B—C59B—C60B—C61B	0.5 (6)	C64D—C59D—C60D—C61D	1.2 (9)
C58B—C59B—C60B—C61B	176.6 (4)	C58D—C59D—C60D—C61D	-178.9 (6)
C59B—C60B—C61B—C62B	0.0 (7)	C59D—C60D—C61D—C62D	-3.1 (11)
C60B—C61B—C62B—C63B	0.3 (7)	C60D—C61D—C62D—C63D	3.4 (11)
C61B—C62B—C63B—C64B	-1.1 (7)	C61D—C62D—C63D—C64D	-2.0 (10)
C60B—C59B—C64B—C63B	-1.4 (6)	C60D—C59D—C64D—C63D	0.2 (8)
C58B—C59B—C64B—C63B	-177.5 (4)	C58D—C59D—C64D—C63D	-179.7 (4)
C62B—C63B—C64B—C59B	1.7 (7)	C62D—C63D—C64D—C59D	0.3 (9)
C25B—O14B—C66B—C67B	-172.8 (3)	C25D—O14D—C66D—C67D	172.7 (3)
C68B—O16B—C67B—O15B	-1.6 (6)	C68D—O16D—C67D—O15D	-4.3 (7)
C68B—O16B—C67B—C66B	-179.6 (4)	C68D—O16D—C67D—C66D	170.9 (4)
O14B—C66B—C67B—O15B	150.2 (4)	O14D—C66D—C67D—O15D	-155.8 (5)
O14B—C66B—C67B—O16B	-31.8 (5)	O14D—C66D—C67D—O16D	28.9 (6)
C26B—C28B—C69B—C70B	-168.7 (3)	C1D—C28D—C69D—C70D	-167.6 (3)
C1B—C28B—C69B—C70B	64.8 (4)	C26D—C28D—C69D—C70D	70.5 (4)
C28B—C69B—C70B—C71B	172.6 (4)	C28D—C69D—C70D—C71D	178.8 (3)

supplementary materials

C69B—C70B—C71B—C76B	104.1 (4)	C69D—C70D—C71D—C72D	-90.2 (5)
C69B—C70B—C71B—C72B	-76.8 (5)	C69D—C70D—C71D—C76D	84.1 (5)
C76B—C71B—C72B—C73B	0.6 (7)	C76D—C71D—C72D—C73D	-1.6 (8)
C70B—C71B—C72B—C73B	-178.5 (4)	C70D—C71D—C72D—C73D	172.8 (5)
C71B—C72B—C73B—C74B	0.5 (8)	C71D—C72D—C73D—C74D	2.0 (10)
C72B—C73B—C74B—C75B	-0.5 (9)	C72D—C73D—C74D—C75D	-1.0 (13)
C73B—C74B—C75B—C76B	-0.5 (8)	C73D—C74D—C75D—C76D	-0.5 (13)
C72B—C71B—C76B—C75B	-1.6 (6)	C74D—C75D—C76D—C71D	0.9 (10)
C70B—C71B—C76B—C75B	177.4 (4)	C72D—C71D—C76D—C75D	0.2 (8)
C74B—C75B—C76B—C71B	1.6 (7)	C70D—C71D—C76D—C75D	-174.3 (5)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C14B—H14B \cdots O16A ⁱ	1.00	2.59	3.440 (4)	142
C30B—H30C \cdots O11A ⁱ	0.99	2.49	3.464 (6)	169
C30C—H30F \cdots O8D ⁱⁱ	0.99	2.55	3.259 (4)	128
C30D—H30G \cdots O8C ⁱⁱⁱ	0.99	2.56	3.270 (5)	129
C44A—H44B \cdots O10B ^{iv}	0.98	2.54	3.292 (5)	133
C56C—H56H \cdots O7B ^v	0.98	2.55	3.375 (9)	141
C56D—H56K \cdots O15A ^{vi}	0.98	2.37	3.251 (8)	149
C62C—H62C \cdots O7C ^{vii}	0.95	2.46	3.313 (6)	149
C62D—H62D \cdots O7D ^{vii}	0.95	2.59	3.421 (7)	146
C63A—H63A \cdots O3B ^{viii}	0.95	2.37	3.267 (7)	156

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, y-1/2, -z+2$; (iii) $-x+1, y+1/2, -z+2$; (iv) $-x+2, y-1/2, -z+1$; (v) $-x+2, y-1/2, -z+2$; (vi) $-x+2, y+1/2, -z+2$; (vii) $x+1, y, z$; (viii) $x-1, y-1, z$.

Fig. 1

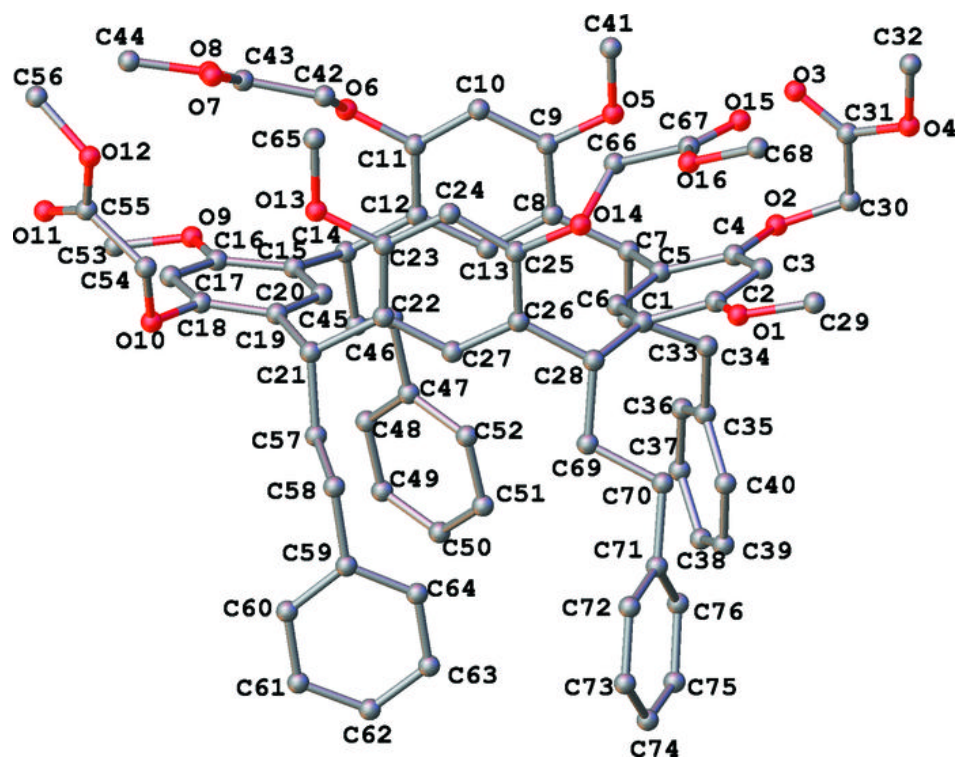


Fig. 2

