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4,4'-Bis[2-(3,5-dimethoxyphenyl)-ethenyl]biphenyl

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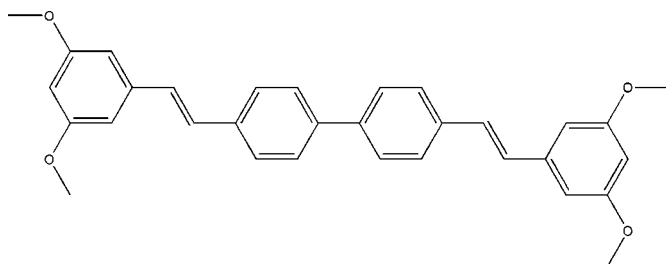
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.060; wR factor = 0.181; data-to-parameter ratio = 18.7.

The title compound, $\text{C}_{32}\text{H}_{30}\text{O}_4$, crystallizes with three different conformers of the same molecule in the asymmetric unit, which explains the unusually large unit cell volume. The supramolecular structure is based on interactions involving the methoxy groups [$\text{C}\cdots\text{O}$ contacts between 3.090 (2) and 3.204 (2) Å, and $\text{C}-\text{H}\cdots\text{O}$ contacts between (normalized) 2.40 and 2.71 Å], $\pi-\pi$ stacking of the electron-rich methoxy-substituted rings [centroid-centroid distances of 3.6454 (9)–3.738 (1) Å] and $\text{C}-\text{H}\cdots\pi$ contacts (normalized, 2.62–2.97 Å).

Related literature

For related methoxy-substituted biphenyls with 4,4'-bis(2-phenylethenyl) substitution, see: Vande Velde *et al.* (2002) [CSD refcode: MODDUE] and Li & Jian (2009) [CSD refcode: POWYUW]. For a study on the blue-light-emitting properties of a related compound, see: Jin *et al.* (2002). For the conformations of methoxybenzenes, see: Vande Velde *et al.* (2007). For the preparation, see: Jin *et al.* (2002).



Experimental

Crystal data

$\text{C}_{32}\text{H}_{30}\text{O}_4$ $V = 7434.8$ (14) Å³
 $M_r = 478.56$ $Z = 12$
 Monoclinic, $P2_1/c$ Mo $K\alpha$ radiation
 $a = 11.8208$ (13) Å $\mu = 0.08$ mm⁻¹
 $b = 27.896$ (3) Å $T = 100$ K
 $c = 22.875$ (3) Å $0.55 \times 0.45 \times 0.15$ mm
 $\beta = 99.723$ (2)°

Data collection

Bruker SMART APEX CCD diffractometer 74405 measured reflections
 Absorption correction: multi-scan (SADABS; Bruker, 2008) 18422 independent reflections
 $T_{\min} = 0.956$, $T_{\max} = 0.988$ 13284 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$ 985 parameters
 $wR(F^2) = 0.181$ H-atom parameters constrained
 $S = 1.03$ $\Delta\rho_{\text{max}} = 0.68$ e Å⁻³
 18422 reflections $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

Table 1

Relevant $\text{C}-\text{H}\cdots\pi$ contacts in the crystal packing of the title compound (Å, °).

$\text{Cg}(X1)$, $\text{Cg}(X2)$, $\text{Cg}(X3)$ and $\text{Cg}(X4)$ are the centroids of the $\text{C}1\text{X}-\text{C}6\text{X}$, $\text{C}9\text{X}-\text{C}14\text{X}$, $\text{C}15\text{X}-\text{C}20\text{X}$ and $\text{C}23\text{X}-\text{C}28\text{X}$ rings, respectively, where $X = A, B, C, D$.

| Entry | D | H | A | H...A | D-H...A |
|-------|------|------|-----------------------|-------|---------|
| 1 | C10A | H10A | $\text{Cg}(B4)^i$ | 2.62 | 148 |
| 2 | C17A | H17A | $\text{Cg}(B3)^i$ | 2.86 | 150 |
| 3 | C19A | H19A | $\text{Cg}(C4)^{ii}$ | 2.80 | 143 |
| 4 | C29A | H29A | $\text{Cg}(A3)^{iii}$ | 2.79 | 147 |
| 5 | C10B | H10B | $\text{Cg}(C1)^{iii}$ | 2.84 | 148 |
| 6 | C14B | H14B | $\text{Cg}(A2)^{iv}$ | 2.97 | 147 |
| 7 | C19B | H19B | $\text{Cg}(A1)^{iv}$ | 2.67 | 149 |
| 8 | C31B | H31B | $\text{Cg}(B2)^{iii}$ | 2.80 | 148 |
| 9 | C10C | H10C | $\text{Cg}(B1)^{iv}$ | 2.70 | 148 |
| 10 | C19C | H19C | $\text{Cg}(A4)^v$ | 2.85 | 152 |
| 11 | C29C | H29C | $\text{Cg}(C3)^i$ | 2.76 | 143 |
| 12 | C31C | H31C | $\text{Cg}(C2)^{iii}$ | 2.78 | 140 |

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

Table 2

Relevant $\pi-\pi$ contacts in the crystal packing of the title compound (Å, °).

The angle related to a pair of centroids is defined as the angle between the $\text{Cg}(I)\cdots\text{Cg}(J)$ vector and the normal to plane I . Centroids as in Table 1.

| Entry | $\text{Cg}(I)$ | $\text{Cg}(J)$ | $\text{Cg}\cdots\text{Cg}$ | Angle |
|-------|-----------------|------------------------|----------------------------|-------|
| 1 | $\text{Cg}(A1)$ | $\text{Cg}(A1)^{vi}$ | 3.738 (1) | 26.65 |
| 2 | $\text{Cg}(A4)$ | $\text{Cg}(A4)^{vii}$ | 3.6454 (9) | 25.18 |
| 3 | $\text{Cg}(B1)$ | $\text{Cg}(C4)^{viii}$ | 3.713 (1) | 25.39 |
| 4 | $\text{Cg}(B4)$ | $\text{Cg}(C1)^{ix}$ | 3.697 (1) | 26.83 |
| 5 | $\text{Cg}(C1)$ | $\text{Cg}(B4)^x$ | 3.697 (1) | 25.86 |
| 6 | $\text{Cg}(C4)$ | $\text{Cg}(B1)^{xi}$ | 3.713 (1) | 25.72 |

Symmetry codes: (vi) $-x, -y + 1, -z$; (vii) $-x + 3, -y + 1, -z + 1$; (viii) $x + 1, -y + \frac{1}{2}, z + \frac{1}{2}$; (ix) $x - 2, -y + \frac{1}{2}, z - \frac{1}{2}$; (x) $x + 2, -y + \frac{1}{2}, z + \frac{1}{2}$; (xi) $x - 1, -y + \frac{1}{2}, z - \frac{1}{2}$.

Table 3

Relevant short contacts involving the methoxy groups in the crystal packing of the title compound (Å, °).

| Entry | D | X | A | $\text{X}\cdots\text{A}$ | $\text{D}-\text{X}\cdots\text{A}$ |
|-------|------|------|--------------------|--------------------------|-----------------------------------|
| 1 | O2A | C30A | O1C ^{ix} | 3.139 (2) | 175.28 (12) |
| 2 | O3A | C31A | O4C ^x | 3.090 (2) | 160.33 (12) |
| 3 | C32A | H32A | O2C ^{vii} | 2.71 | 120 |
| 4 | C32A | H32c | O3A ^{vii} | 2.55 | 142 |
| 5 | C15B | C16B | O1B ⁱⁱⁱ | 3.204 (2) | 108.54 (9) |
| 6 | O1B | C29B | O4A ^{vii} | 3.171 (2) | 143.57 (12) |
| 7 | O2B | C30B | O3B ^v | 3.171 (2) | 171.88 (12) |
| 8 | O4B | C32B | O1A ^{xii} | 3.102 (2) | 174.13 (12) |
| 9 | C31B | H31D | O2C ^{ix} | 2.68 | 139 |

| Entry | <i>D</i> | <i>X</i> | <i>A</i> | <i>X</i> ··· <i>A</i> | <i>D</i> – <i>X</i> ··· <i>A</i> |
|-------|--------------|--------------|-----------------------------|-----------------------|----------------------------------|
| 10 | O2 <i>C</i> | C30 <i>C</i> | O3 <i>C</i> ^x | 3.152 (2) | 161.25 (11) |
| 11 | C29 <i>C</i> | H29 <i>H</i> | O4 <i>B</i> ^x | 2.67 | 141 |
| 12 | C31 <i>C</i> | H31 <i>I</i> | O2 <i>B</i> ^{xi} | 2.70 | 143 |
| 13 | C32 <i>C</i> | H32 <i>G</i> | O1 <i>B</i> ^{xi} | 2.40 | 144 |
| 14 | C32 <i>C</i> | H32 <i>I</i> | O4 <i>C</i> ^{xiii} | 2.69 | 124 |

Symmetry codes: (xii) $-x - 1, -y + 1, -z$; (xiii) $-x, -y, -z$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINTE* (Bruker, 2008); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2079).

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supporting information

Acta Cryst. (2011). E67, o1112–o1113 [doi:10.1107/S1600536811012888]

4,4'-Bis[2-(3,5-dimethoxyphenyl)ethenyl]biphenyl

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S1. Comment

The title compound was synthesized with its use as the active component in an organic blue-light-emitting diode in mind (Jin *et al.*, 2002). Three conformers of the same molecule are present in the asymmetric unit, displaying different conformations of the methoxy groups and the biphenyl moiety; the molecules have been labeled A, B and C and the numbering scheme is given in Fig. 1. Fig. 2 presents a packing diagram. Molecules A and B have non-planar biphenyl units, with dihedral angles of 30.97 (7)° and 30.51 (7)°, respectively, while the same moiety in molecule C is virtually planar [4.22 (8)°]. In each of the three molecules the methoxy groups are oriented differently: their precise orientations do not have a large influence on the relative stability of the conformer (Vande Velde *et al.*, 2007) but are merely due to the intermolecular contacts they are involved in. The three crystallographically independent molecules are held together by three C–H··· π interactions involving aromatic hydrogen atoms. Rings 1 and 2 of molecule A are contacted by H14B and H19B (Table 1, entries 6 and 7) and ring 1 of molecule B is contacted by H10C (Table 1, entry 9). Additionally, molecule A is involved in two methoxy···methoxy contacts (Table 3, entries 1 and 2), two C–H···O contacts involving the methoxy group in the 3-position (Table 3, entries 3 and 4), four C–H··· π interactions involving aromatic hydrogen atoms (Table 1, entries 1–4) and two π – π contacts with a symmetry-related A molecule (Table 2, entries 1 and 2). The supramolecular organization of molecule B is based on four methoxy···methoxy contacts (Table 3, entries 5–8), one contact involving the hydrogen atoms of the methoxy group in the 3-position (Table 3, entry 9), two additional C–H··· π interactions (Table 1, entries 5 and 8) and two π – π contacts involving the methoxy-substituted rings (1 and 4) of molecules B and C (Table 2, entries 3 and 4). Molecule C participates in five contacts involving the methoxy groups, of which one is a methoxy···methoxy contact (Table 3, entry 10) and four are initiated by hydrogen atoms of the methoxy groups (Table 3, entries 11–14). Two contacts involve the π -systems of the methoxy-substituted rings of molecules B and C (Table 2, entries 5 and 6). Finally, it can be clearly seen from Table 2 that all three molecules are engaged in π – π stacking of the electron-rich methoxy-substituted rings 1 and 4.

S2. Experimental

The title compound was prepared as is outlined in Yin *et al.* (2002). Crystals suitable for the diffraction experiment were grown by slow evaporation of an acetone solution. *M.p.* (uncorrected) 452 K. ¹H NMR (CDCl₃, 400 MHz, TMS): δ 3.83 (s, OCH₃), 6.41 (t, 2.2 Hz, H4, H26), 6.69 (d, 2.2 Hz, H2, H6, H24, H28), 7.06 (d, 16.3 Hz, H7/H22 or H8/H21), 7.11 (d, 16.3 Hz, H7/H22 or H8/H21), 7.56 (d, 8.4 Hz, H10, H14, H17, H19), 7.61 (d, 8.4 Hz, H11, H13, H17, H19) p.p.m. ¹³C NMR (CDCl₃, 100 MHz, TMS): δ 55.40 (C29, C30, C31, C32), 100.12 (C4, C26), 104.69 (C2, C6, C24, C28), 127.08 (C10, C14, C17, C19), 127.09 (C11, C13, C16, C20), 128.71 (C7/C22 or C8/C21), 128.81 (C7/C22 or C8/C21), 136.32 (C9, C18), 139.38 (C12, C15), 139.83 (C1, C23), 161.06 (C3, C5, C25, C27) p.p.m.

S3. Refinement

Hydrogen atoms were placed in calculated positions and refined as riding with C—H distances of 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

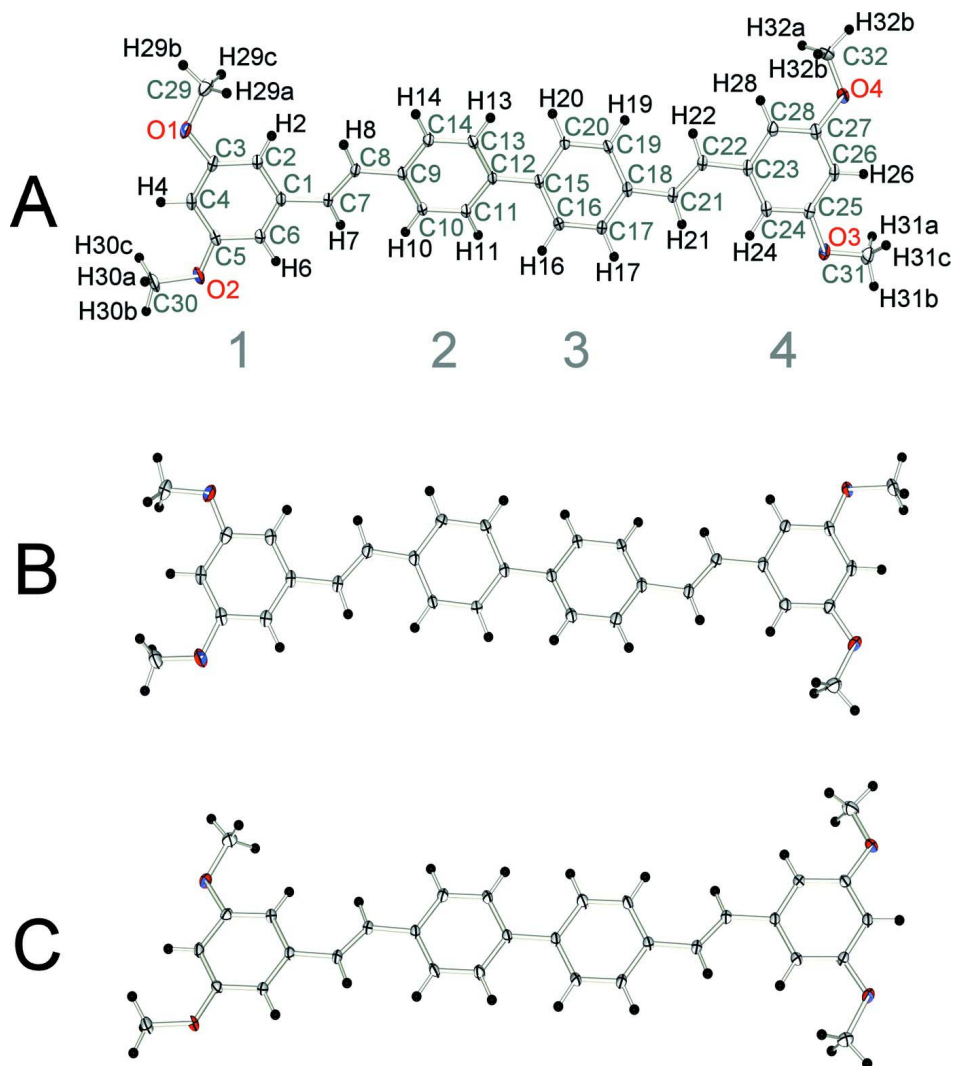
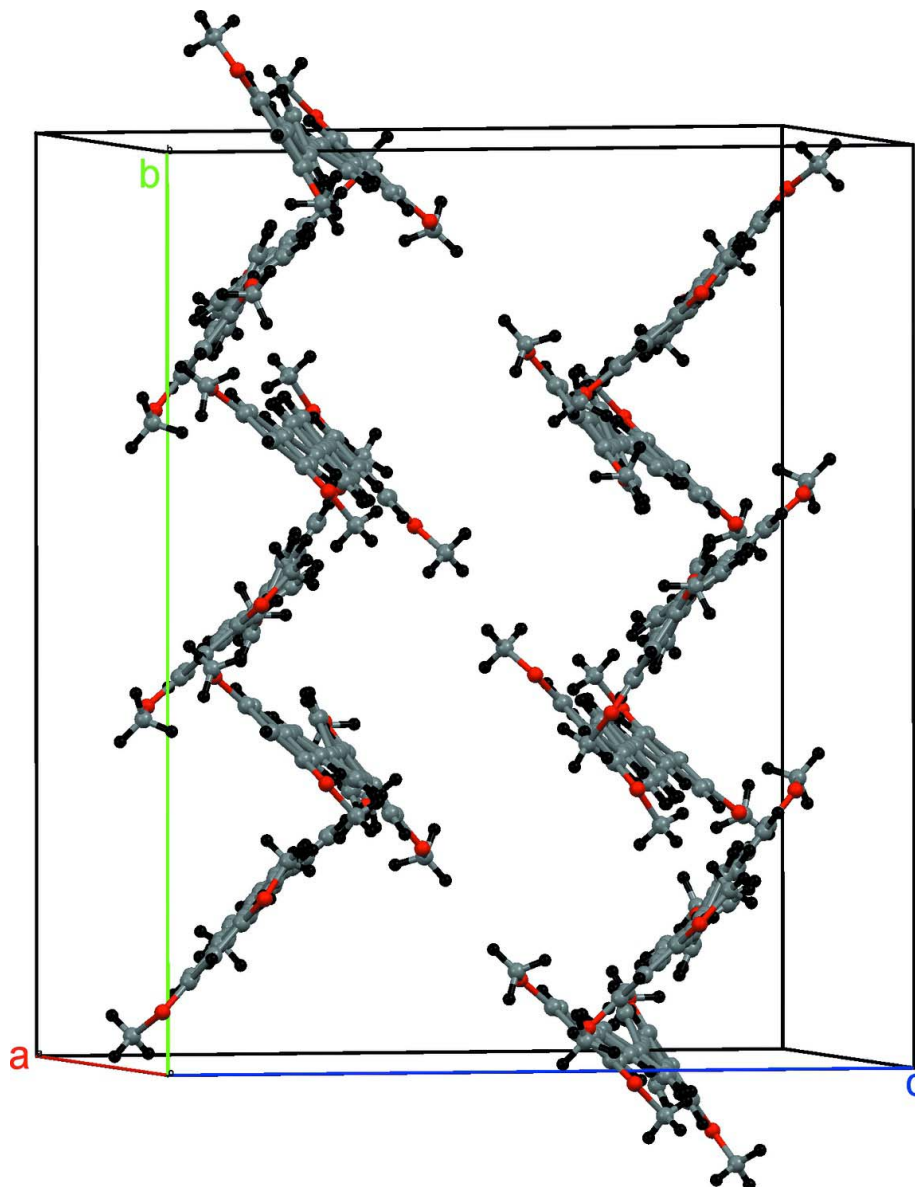


Figure 1

Molecular structure of the title compound showing the numbering scheme of the three crystallographically independent molecules (A, B, C). Displacement ellipsoids are drawn at the 50% probability level; hydrogen atoms are represented by spheres with an arbitrary radius. Hydrogen atoms of methoxy groups are denominated with a lower case suffix: a, b, c for A, d, e, f for B, and g, h, i for C.

**Figure 2**

Packing scheme of the title compound.

4,4'-Bis[2-(3,5-dimethoxyphenyl)ethenyl]biphenyl

Crystal data

$C_{32}H_{30}O_4$

$M_r = 478.56$

Monoclinic, $P2_1/c$

Hall symbol: $-P 2_1/c$

$a = 11.8208 (13) \text{ \AA}$

$b = 27.896 (3) \text{ \AA}$

$c = 22.875 (3) \text{ \AA}$

$\beta = 99.723 (2)^\circ$

$V = 7434.8 (14) \text{ \AA}^3$

$Z = 12$

$F(000) = 3048$

$D_x = 1.283 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 9749 reflections

$\theta = 2.3\text{--}32.8^\circ$

$\mu = 0.08 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Plate, colourless

$0.55 \times 0.45 \times 0.15 \text{ mm}$

Data collection

| | |
|--|--|
| Bruker SMART APEX CCD diffractometer | 74405 measured reflections |
| Radiation source: fine-focus sealed tube | 18422 independent reflections |
| Graphite monochromator | 13284 reflections with $I > 2\sigma(I)$ |
| ω scans | $R_{\text{int}} = 0.034$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2008) | $\theta_{\text{max}} = 28.3^\circ$, $\theta_{\text{min}} = 1.7^\circ$ |
| $T_{\text{min}} = 0.956$, $T_{\text{max}} = 0.988$ | $h = -15 \rightarrow 15$ |
| | $k = -37 \rightarrow 37$ |
| | $l = -30 \rightarrow 30$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.060$ | H-atom parameters constrained |
| $wR(F^2) = 0.181$ | $w = 1/[\sigma^2(F_o^2) + (0.0954P)^2 + 3.3183P]$ |
| $S = 1.03$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 18422 reflections | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 985 parameters | $\Delta\rho_{\text{max}} = 0.68 \text{ e } \text{\AA}^{-3}$ |
| 0 restraints | $\Delta\rho_{\text{min}} = -0.29 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | |

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ 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. The data has been truncated at 0.75 Å.

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|-------------|-------------|----------------------------------|
| C1A | 0.15447 (12) | 0.46499 (5) | 0.09560 (6) | 0.0168 (3) |
| C2A | 0.06813 (12) | 0.49166 (5) | 0.11557 (6) | 0.0174 (3) |
| H2A | 0.0861 | 0.5124 | 0.1488 | 0.021* |
| C3A | -0.04359 (12) | 0.48741 (5) | 0.08623 (7) | 0.0181 (3) |
| C4A | -0.07196 (12) | 0.45719 (5) | 0.03724 (7) | 0.0188 (3) |
| H4A | -0.1490 | 0.4549 | 0.0172 | 0.023* |
| C5A | 0.01347 (12) | 0.43065 (5) | 0.01832 (7) | 0.0188 (3) |
| C6A | 0.12663 (12) | 0.43462 (5) | 0.04730 (7) | 0.0193 (3) |
| H6A | 0.1851 | 0.4164 | 0.0339 | 0.023* |
| C7A | 0.27507 (12) | 0.46747 (5) | 0.12364 (7) | 0.0180 (3) |
| H7A | 0.3278 | 0.4508 | 0.1040 | 0.022* |
| C8A | 0.32024 (12) | 0.49024 (5) | 0.17333 (6) | 0.0155 (3) |
| H8A | 0.2692 | 0.5069 | 0.1941 | 0.019* |
| C9A | 0.44267 (12) | 0.49152 (5) | 0.19832 (6) | 0.0147 (3) |
| C10A | 0.52534 (12) | 0.46805 (5) | 0.17172 (7) | 0.0184 (3) |

| | | | | |
|------|---------------|-------------|--------------|------------|
| H10A | 0.5020 | 0.4505 | 0.1361 | 0.022* |
| C11A | 0.63999 (12) | 0.46991 (5) | 0.19625 (7) | 0.0188 (3) |
| H11A | 0.6942 | 0.4537 | 0.1771 | 0.023* |
| C12A | 0.67846 (12) | 0.49502 (5) | 0.24851 (6) | 0.0145 (3) |
| C13A | 0.59664 (12) | 0.51896 (5) | 0.27477 (6) | 0.0179 (3) |
| H13A | 0.6202 | 0.5369 | 0.3101 | 0.021* |
| C14A | 0.48114 (12) | 0.51703 (5) | 0.25009 (6) | 0.0175 (3) |
| H14A | 0.4270 | 0.5335 | 0.2690 | 0.021* |
| C15A | 0.80193 (12) | 0.49572 (5) | 0.27384 (6) | 0.0153 (3) |
| C16A | 0.87267 (13) | 0.45705 (6) | 0.26583 (7) | 0.0223 (3) |
| H16A | 0.8399 | 0.4293 | 0.2455 | 0.027* |
| C17A | 0.98942 (13) | 0.45819 (6) | 0.28679 (7) | 0.0236 (3) |
| H17A | 1.0354 | 0.4315 | 0.2801 | 0.028* |
| C18A | 1.04088 (12) | 0.49784 (5) | 0.31748 (6) | 0.0175 (3) |
| C19A | 0.96978 (12) | 0.53637 (5) | 0.32649 (6) | 0.0160 (3) |
| H19A | 1.0022 | 0.5638 | 0.3477 | 0.019* |
| C20A | 0.85324 (12) | 0.53519 (5) | 0.30507 (6) | 0.0150 (3) |
| H20A | 0.8071 | 0.5619 | 0.3118 | 0.018* |
| C21A | 1.16440 (12) | 0.49687 (6) | 0.34026 (7) | 0.0197 (3) |
| H21A | 1.2078 | 0.4722 | 0.3258 | 0.024* |
| C22A | 1.22132 (12) | 0.52726 (5) | 0.37928 (6) | 0.0178 (3) |
| H22A | 1.1775 | 0.5521 | 0.3930 | 0.021* |
| C23A | 1.34420 (12) | 0.52665 (5) | 0.40355 (6) | 0.0167 (3) |
| C24A | 1.41857 (12) | 0.49137 (6) | 0.39001 (6) | 0.0189 (3) |
| H24A | 1.3902 | 0.4657 | 0.3643 | 0.023* |
| C25A | 1.53484 (12) | 0.49360 (6) | 0.41414 (7) | 0.0187 (3) |
| C26A | 1.57761 (12) | 0.53051 (5) | 0.45167 (6) | 0.0184 (3) |
| H26A | 1.6571 | 0.5320 | 0.4678 | 0.022* |
| C27A | 1.50255 (12) | 0.56549 (5) | 0.46552 (6) | 0.0180 (3) |
| C28A | 1.38688 (12) | 0.56404 (5) | 0.44188 (6) | 0.0179 (3) |
| H28A | 1.3367 | 0.5883 | 0.4516 | 0.021* |
| C29A | -0.10905 (14) | 0.54661 (7) | 0.14674 (7) | 0.0280 (4) |
| H29A | -0.0678 | 0.5318 | 0.1830 | 0.042* |
| H29B | -0.1807 | 0.5608 | 0.1548 | 0.042* |
| H29C | -0.0612 | 0.5716 | 0.1334 | 0.042* |
| C30A | -0.11888 (14) | 0.38859 (7) | -0.05346 (8) | 0.0342 (4) |
| H30A | -0.1587 | 0.3759 | -0.0225 | 0.051* |
| H30B | -0.1196 | 0.3645 | -0.0847 | 0.051* |
| H30C | -0.1579 | 0.4177 | -0.0704 | 0.051* |
| C31A | 1.72111 (13) | 0.45930 (7) | 0.41990 (8) | 0.0301 (4) |
| H31A | 1.7529 | 0.4888 | 0.4060 | 0.045* |
| H31B | 1.7582 | 0.4315 | 0.4050 | 0.045* |
| H31C | 1.7350 | 0.4588 | 0.4634 | 0.045* |
| C32A | 1.47986 (15) | 0.63504 (6) | 0.52207 (9) | 0.0330 (4) |
| H32A | 1.4360 | 0.6513 | 0.4876 | 0.050* |
| H32B | 1.5262 | 0.6586 | 0.5474 | 0.050* |
| H32C | 1.4269 | 0.6192 | 0.5446 | 0.050* |
| C29B | 1.22529 (13) | 0.35012 (7) | 0.42489 (8) | 0.0291 (4) |

| | | | | |
|------|---------------|-------------|-------------|------------|
| H29D | 1.2407 | 0.3509 | 0.4683 | 0.044* |
| H29E | 1.2680 | 0.3759 | 0.4093 | 0.044* |
| H29F | 1.2496 | 0.3191 | 0.4110 | 0.044* |
| C2B | 0.91825 (13) | 0.32978 (6) | 0.39548 (7) | 0.0194 (3) |
| H2B | 0.8969 | 0.3547 | 0.3675 | 0.023* |
| C3B | 1.03183 (13) | 0.32419 (6) | 0.42179 (7) | 0.0199 (3) |
| C4B | 1.06591 (13) | 0.28789 (6) | 0.46322 (7) | 0.0202 (3) |
| H4B | 1.1441 | 0.2844 | 0.4810 | 0.024* |
| C5B | 0.98301 (13) | 0.25722 (6) | 0.47757 (7) | 0.0205 (3) |
| C6B | 0.86925 (13) | 0.26214 (6) | 0.45118 (7) | 0.0201 (3) |
| H6B | 0.8135 | 0.2404 | 0.4610 | 0.024* |
| C1B | 0.83559 (12) | 0.29863 (5) | 0.41031 (6) | 0.0181 (3) |
| C7B | 0.71374 (12) | 0.30156 (6) | 0.38449 (6) | 0.0186 (3) |
| H7B | 0.6658 | 0.2776 | 0.3968 | 0.022* |
| C8B | 0.66159 (12) | 0.33367 (5) | 0.34585 (7) | 0.0192 (3) |
| H8B | 0.7080 | 0.3580 | 0.3330 | 0.023* |
| C9B | 0.53876 (12) | 0.33459 (5) | 0.32160 (6) | 0.0176 (3) |
| C10B | 0.46492 (12) | 0.29667 (5) | 0.32902 (6) | 0.0166 (3) |
| H10B | 0.4946 | 0.2691 | 0.3507 | 0.020* |
| C11B | 0.34943 (12) | 0.29875 (5) | 0.30531 (6) | 0.0156 (3) |
| H11B | 0.3014 | 0.2724 | 0.3109 | 0.019* |
| C12B | 0.30172 (12) | 0.33866 (5) | 0.27328 (6) | 0.0161 (3) |
| C13B | 0.37525 (13) | 0.37678 (6) | 0.26680 (7) | 0.0212 (3) |
| H13B | 0.3452 | 0.4047 | 0.2460 | 0.025* |
| C14B | 0.49105 (13) | 0.37460 (6) | 0.29016 (7) | 0.0225 (3) |
| H14B | 0.5391 | 0.4010 | 0.2847 | 0.027* |
| C15B | 0.17901 (12) | 0.34021 (5) | 0.24667 (6) | 0.0163 (3) |
| C16B | 0.09571 (12) | 0.31668 (5) | 0.27237 (7) | 0.0189 (3) |
| H16B | 0.1181 | 0.2985 | 0.3075 | 0.023* |
| C17B | -0.01938 (12) | 0.31947 (6) | 0.24737 (7) | 0.0197 (3) |
| H17B | -0.0745 | 0.3032 | 0.2659 | 0.024* |
| C18B | -0.05605 (12) | 0.34550 (5) | 0.19575 (7) | 0.0170 (3) |
| C19B | 0.02796 (12) | 0.36855 (5) | 0.16970 (7) | 0.0186 (3) |
| H19B | 0.0057 | 0.3863 | 0.1342 | 0.022* |
| C20B | 0.14264 (12) | 0.36598 (5) | 0.19463 (7) | 0.0182 (3) |
| H20B | 0.1978 | 0.3821 | 0.1760 | 0.022* |
| C21B | -0.17861 (12) | 0.34744 (5) | 0.17100 (7) | 0.0184 (3) |
| H21B | -0.2294 | 0.3295 | 0.1906 | 0.022* |
| C22B | -0.22425 (12) | 0.37232 (5) | 0.12328 (7) | 0.0192 (3) |
| H22B | -0.1721 | 0.3903 | 0.1047 | 0.023* |
| C23B | -0.34536 (12) | 0.37534 (5) | 0.09590 (7) | 0.0173 (3) |
| C24B | -0.43179 (12) | 0.34840 (5) | 0.11558 (7) | 0.0183 (3) |
| H24B | -0.4137 | 0.3275 | 0.1487 | 0.022* |
| C25B | -0.54361 (12) | 0.35257 (5) | 0.08623 (7) | 0.0177 (3) |
| C26B | -0.57203 (12) | 0.38340 (5) | 0.03787 (7) | 0.0174 (3) |
| H26B | -0.6490 | 0.3856 | 0.0176 | 0.021* |
| C27B | -0.48670 (12) | 0.41062 (5) | 0.01991 (6) | 0.0169 (3) |
| C28B | -0.37355 (12) | 0.40639 (5) | 0.04856 (7) | 0.0180 (3) |

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|------|---------------|-------------|--------------|------------|
| H28B | -0.3152 | 0.4250 | 0.0355 | 0.022* |
| C30B | 1.12008 (15) | 0.20950 (7) | 0.54112 (8) | 0.0331 (4) |
| H30D | 1.1599 | 0.1998 | 0.5087 | 0.050* |
| H30E | 1.1228 | 0.1832 | 0.5697 | 0.050* |
| H30F | 1.1577 | 0.2378 | 0.5609 | 0.050* |
| C31B | -0.60962 (15) | 0.29225 (6) | 0.14510 (8) | 0.0283 (4) |
| H31D | -0.5607 | 0.2677 | 0.1316 | 0.042* |
| H31E | -0.6814 | 0.2776 | 0.1523 | 0.042* |
| H31F | -0.5697 | 0.3067 | 0.1819 | 0.042* |
| C32B | -0.62030 (14) | 0.45357 (7) | -0.04972 (8) | 0.0294 (4) |
| H32D | -0.6592 | 0.4247 | -0.0674 | 0.044* |
| H32E | -0.6222 | 0.4784 | -0.0802 | 0.044* |
| H32F | -0.6594 | 0.4653 | -0.0180 | 0.044* |
| C6C | 1.38454 (12) | 0.22574 (5) | 0.45759 (6) | 0.0158 (3) |
| H6C | 1.3298 | 0.2449 | 0.4729 | 0.019* |
| C5C | 1.49943 (12) | 0.22673 (5) | 0.48485 (6) | 0.0160 (3) |
| C4C | 1.57998 (12) | 0.19932 (5) | 0.46280 (7) | 0.0171 (3) |
| H4C | 1.6584 | 0.2001 | 0.4811 | 0.021* |
| C3C | 1.54444 (12) | 0.17039 (5) | 0.41322 (7) | 0.0168 (3) |
| C2C | 1.43104 (12) | 0.16884 (5) | 0.38582 (6) | 0.0165 (3) |
| H2C | 1.4083 | 0.1490 | 0.3521 | 0.020* |
| C1C | 1.34976 (12) | 0.19700 (5) | 0.40838 (6) | 0.0151 (3) |
| C7C | 1.22788 (12) | 0.19699 (5) | 0.38199 (6) | 0.0164 (3) |
| H7C | 1.1789 | 0.2163 | 0.4011 | 0.020* |
| C8C | 1.17803 (12) | 0.17304 (5) | 0.33432 (6) | 0.0167 (3) |
| H8C | 1.2263 | 0.1541 | 0.3143 | 0.020* |
| C9C | 1.05527 (12) | 0.17327 (5) | 0.31000 (6) | 0.0151 (3) |
| C14C | 1.01218 (13) | 0.14143 (6) | 0.26500 (8) | 0.0264 (4) |
| H14C | 1.0635 | 0.1204 | 0.2499 | 0.032* |
| C13C | 0.89656 (14) | 0.13968 (6) | 0.24167 (8) | 0.0286 (4) |
| H13C | 0.8701 | 0.1172 | 0.2112 | 0.034* |
| C12C | 0.81788 (12) | 0.17009 (5) | 0.26172 (6) | 0.0151 (3) |
| C11C | 0.86161 (12) | 0.20175 (6) | 0.30668 (7) | 0.0212 (3) |
| H11C | 0.8104 | 0.2229 | 0.3217 | 0.025* |
| C10C | 0.97666 (13) | 0.20354 (6) | 0.33027 (7) | 0.0212 (3) |
| H10C | 1.0029 | 0.2259 | 0.3609 | 0.025* |
| C15C | 0.69448 (12) | 0.16939 (5) | 0.23627 (6) | 0.0154 (3) |
| C20C | 0.64884 (13) | 0.13538 (6) | 0.19423 (7) | 0.0231 (3) |
| H20C | 0.6990 | 0.1129 | 0.1808 | 0.028* |
| C19C | 0.53336 (13) | 0.13335 (6) | 0.17159 (7) | 0.0238 (3) |
| H19C | 0.5059 | 0.1096 | 0.1430 | 0.029* |
| C18C | 0.45600 (12) | 0.16546 (5) | 0.18980 (6) | 0.0162 (3) |
| C17C | 0.50090 (14) | 0.19927 (6) | 0.23188 (8) | 0.0291 (4) |
| H17C | 0.4505 | 0.2214 | 0.2459 | 0.035* |
| C16C | 0.61719 (14) | 0.20155 (6) | 0.25398 (8) | 0.0309 (4) |
| H16C | 0.6449 | 0.2257 | 0.2820 | 0.037* |
| C21C | 0.33291 (12) | 0.16459 (5) | 0.16694 (6) | 0.0172 (3) |
| H21C | 0.2852 | 0.1838 | 0.1870 | 0.021* |

| | | | | |
|------|---------------|-------------|--------------|------------|
| C22C | 0.28167 (12) | 0.13947 (5) | 0.12067 (6) | 0.0168 (3) |
| H22C | 0.3301 | 0.1205 | 0.1009 | 0.020* |
| C23C | 0.15881 (12) | 0.13783 (5) | 0.09682 (6) | 0.0150 (3) |
| C28C | 0.12162 (12) | 0.10430 (5) | 0.05276 (6) | 0.0161 (3) |
| H28C | 0.1754 | 0.0836 | 0.0390 | 0.019* |
| C27C | 0.00576 (12) | 0.10107 (5) | 0.02884 (6) | 0.0162 (3) |
| C26C | -0.07309 (12) | 0.13105 (5) | 0.04851 (6) | 0.0163 (3) |
| H26C | -0.1523 | 0.1287 | 0.0322 | 0.020* |
| C25C | -0.03562 (12) | 0.16461 (5) | 0.09225 (6) | 0.0162 (3) |
| C24C | 0.07974 (12) | 0.16824 (5) | 0.11681 (6) | 0.0170 (3) |
| H24C | 0.1046 | 0.1912 | 0.1469 | 0.020* |
| C30C | 1.64021 (13) | 0.26068 (6) | 0.56038 (8) | 0.0260 (3) |
| H30G | 1.6725 | 0.2292 | 0.5727 | 0.039* |
| H30H | 1.6454 | 0.2816 | 0.5951 | 0.039* |
| H30I | 1.6834 | 0.2749 | 0.5317 | 0.039* |
| C29C | 1.59720 (14) | 0.10730 (6) | 0.35327 (7) | 0.0259 (3) |
| H29G | 1.5527 | 0.1209 | 0.3171 | 0.039* |
| H29H | 1.5502 | 0.0838 | 0.3701 | 0.039* |
| H29I | 1.6660 | 0.0916 | 0.3438 | 0.039* |
| C32C | 0.04090 (15) | 0.04176 (6) | -0.04099 (8) | 0.0279 (4) |
| H32G | 0.0907 | 0.0634 | -0.0589 | 0.042* |
| H32H | -0.0014 | 0.0210 | -0.0717 | 0.042* |
| H32I | 0.0878 | 0.0220 | -0.0108 | 0.042* |
| C31C | -0.08460 (14) | 0.23222 (6) | 0.14598 (8) | 0.0277 (4) |
| H31G | -0.0384 | 0.2209 | 0.1831 | 0.042* |
| H31H | -0.1526 | 0.2491 | 0.1547 | 0.042* |
| H31I | -0.0387 | 0.2541 | 0.1260 | 0.042* |
| O1A | -0.13450 (9) | 0.51116 (4) | 0.10185 (5) | 0.0246 (3) |
| O2A | -0.00321 (9) | 0.39978 (4) | -0.02838 (5) | 0.0269 (3) |
| O3A | 1.60083 (9) | 0.45756 (4) | 0.39861 (5) | 0.0257 (3) |
| O4A | 1.55294 (9) | 0.60032 (4) | 0.50278 (5) | 0.0261 (3) |
| O1B | 1.10602 (9) | 0.35647 (4) | 0.40456 (5) | 0.0259 (3) |
| O2B | 1.00406 (10) | 0.22052 (5) | 0.51787 (5) | 0.0301 (3) |
| O3B | -0.63448 (9) | 0.32819 (4) | 0.10092 (5) | 0.0261 (3) |
| O4B | -0.50431 (9) | 0.44240 (4) | -0.02580 (5) | 0.0232 (2) |
| O2C | 1.52291 (9) | 0.25537 (4) | 0.53358 (5) | 0.0210 (2) |
| O1C | 1.63029 (9) | 0.14468 (4) | 0.39530 (5) | 0.0232 (2) |
| O4C | -0.03835 (9) | 0.06925 (4) | -0.01410 (5) | 0.0233 (2) |
| O3C | -0.11947 (9) | 0.19248 (4) | 0.10853 (5) | 0.0239 (2) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|------------|-------------|-------------|-------------|
| C1A | 0.0112 (6) | 0.0184 (7) | 0.0195 (7) | -0.0013 (5) | -0.0009 (5) | 0.0008 (5) |
| C2A | 0.0129 (7) | 0.0200 (7) | 0.0181 (7) | -0.0001 (5) | -0.0005 (5) | -0.0009 (6) |
| C3A | 0.0114 (7) | 0.0224 (7) | 0.0201 (7) | 0.0019 (5) | 0.0014 (5) | 0.0044 (6) |
| C4A | 0.0115 (6) | 0.0239 (7) | 0.0199 (7) | -0.0029 (5) | -0.0005 (5) | 0.0034 (6) |
| C5A | 0.0150 (7) | 0.0221 (7) | 0.0184 (7) | -0.0056 (6) | -0.0001 (5) | -0.0013 (6) |

| | | | | | | |
|------|------------|-------------|-------------|-------------|-------------|-------------|
| C6A | 0.0124 (7) | 0.0210 (7) | 0.0241 (8) | -0.0015 (5) | 0.0019 (6) | -0.0038 (6) |
| C7A | 0.0108 (6) | 0.0191 (7) | 0.0228 (7) | 0.0006 (5) | -0.0008 (5) | -0.0028 (6) |
| C8A | 0.0105 (6) | 0.0164 (7) | 0.0188 (7) | 0.0002 (5) | 0.0005 (5) | 0.0020 (5) |
| C9A | 0.0115 (6) | 0.0144 (6) | 0.0171 (7) | -0.0022 (5) | -0.0009 (5) | 0.0024 (5) |
| C10A | 0.0133 (7) | 0.0202 (7) | 0.0201 (7) | 0.0000 (5) | -0.0019 (5) | -0.0056 (6) |
| C11A | 0.0119 (7) | 0.0214 (7) | 0.0221 (7) | 0.0004 (5) | -0.0001 (5) | -0.0059 (6) |
| C12A | 0.0108 (6) | 0.0150 (6) | 0.0166 (7) | -0.0014 (5) | -0.0012 (5) | 0.0007 (5) |
| C13A | 0.0145 (7) | 0.0212 (7) | 0.0168 (7) | -0.0019 (5) | -0.0006 (5) | -0.0044 (6) |
| C14A | 0.0126 (7) | 0.0215 (7) | 0.0181 (7) | 0.0004 (5) | 0.0017 (5) | -0.0017 (6) |
| C15A | 0.0118 (6) | 0.0178 (7) | 0.0151 (6) | -0.0022 (5) | -0.0015 (5) | -0.0004 (5) |
| C16A | 0.0154 (7) | 0.0201 (7) | 0.0285 (8) | 0.0006 (6) | -0.0046 (6) | -0.0081 (6) |
| C17A | 0.0149 (7) | 0.0228 (8) | 0.0301 (8) | 0.0034 (6) | -0.0048 (6) | -0.0078 (6) |
| C18A | 0.0135 (7) | 0.0212 (7) | 0.0163 (7) | -0.0018 (5) | -0.0019 (5) | 0.0008 (5) |
| C19A | 0.0146 (7) | 0.0168 (7) | 0.0150 (6) | -0.0033 (5) | -0.0020 (5) | -0.0005 (5) |
| C20A | 0.0131 (7) | 0.0159 (7) | 0.0150 (6) | -0.0001 (5) | -0.0003 (5) | -0.0001 (5) |
| C21A | 0.0124 (7) | 0.0235 (8) | 0.0219 (7) | 0.0008 (6) | -0.0011 (6) | -0.0007 (6) |
| C22A | 0.0121 (7) | 0.0214 (7) | 0.0187 (7) | -0.0006 (5) | -0.0007 (5) | 0.0023 (6) |
| C23A | 0.0128 (7) | 0.0213 (7) | 0.0150 (7) | -0.0025 (5) | -0.0005 (5) | 0.0049 (5) |
| C24A | 0.0150 (7) | 0.0230 (7) | 0.0172 (7) | -0.0023 (6) | -0.0014 (5) | 0.0012 (6) |
| C25A | 0.0152 (7) | 0.0224 (7) | 0.0182 (7) | 0.0007 (6) | 0.0018 (5) | 0.0044 (6) |
| C26A | 0.0122 (7) | 0.0233 (7) | 0.0183 (7) | -0.0035 (5) | -0.0015 (5) | 0.0069 (6) |
| C27A | 0.0166 (7) | 0.0186 (7) | 0.0173 (7) | -0.0044 (5) | -0.0015 (5) | 0.0055 (5) |
| C28A | 0.0156 (7) | 0.0182 (7) | 0.0187 (7) | -0.0008 (5) | -0.0005 (5) | 0.0042 (6) |
| C29A | 0.0231 (8) | 0.0379 (10) | 0.0228 (8) | 0.0110 (7) | 0.0036 (6) | -0.0032 (7) |
| C30A | 0.0205 (8) | 0.0429 (11) | 0.0360 (10) | -0.0110 (7) | -0.0046 (7) | -0.0150 (8) |
| C31A | 0.0162 (8) | 0.0386 (10) | 0.0345 (9) | 0.0034 (7) | 0.0014 (7) | -0.0026 (8) |
| C32A | 0.0286 (9) | 0.0219 (8) | 0.0447 (11) | -0.0001 (7) | -0.0052 (8) | -0.0094 (7) |
| C29B | 0.0162 (8) | 0.0372 (10) | 0.0333 (9) | -0.0027 (7) | 0.0027 (7) | -0.0052 (7) |
| C2B | 0.0172 (7) | 0.0223 (7) | 0.0175 (7) | 0.0014 (6) | -0.0007 (6) | -0.0021 (6) |
| C3B | 0.0161 (7) | 0.0232 (7) | 0.0203 (7) | -0.0014 (6) | 0.0028 (6) | -0.0080 (6) |
| C4B | 0.0135 (7) | 0.0273 (8) | 0.0186 (7) | 0.0036 (6) | -0.0006 (5) | -0.0069 (6) |
| C5B | 0.0172 (7) | 0.0248 (8) | 0.0183 (7) | 0.0049 (6) | -0.0001 (6) | -0.0024 (6) |
| C6B | 0.0156 (7) | 0.0238 (8) | 0.0205 (7) | 0.0011 (6) | 0.0016 (6) | -0.0021 (6) |
| C1B | 0.0131 (7) | 0.0225 (7) | 0.0172 (7) | 0.0027 (5) | -0.0015 (5) | -0.0045 (6) |
| C7B | 0.0126 (7) | 0.0231 (7) | 0.0191 (7) | 0.0008 (5) | -0.0004 (5) | -0.0023 (6) |
| C8B | 0.0146 (7) | 0.0204 (7) | 0.0212 (7) | -0.0009 (5) | -0.0013 (6) | -0.0020 (6) |
| C9B | 0.0148 (7) | 0.0192 (7) | 0.0174 (7) | 0.0009 (5) | -0.0017 (5) | -0.0017 (5) |
| C10B | 0.0137 (7) | 0.0167 (7) | 0.0176 (7) | 0.0027 (5) | -0.0023 (5) | 0.0004 (5) |
| C11B | 0.0145 (7) | 0.0153 (7) | 0.0167 (7) | 0.0000 (5) | 0.0014 (5) | 0.0008 (5) |
| C12B | 0.0135 (7) | 0.0184 (7) | 0.0150 (6) | 0.0016 (5) | -0.0016 (5) | -0.0007 (5) |
| C13B | 0.0175 (7) | 0.0182 (7) | 0.0251 (8) | 0.0008 (6) | -0.0043 (6) | 0.0042 (6) |
| C14B | 0.0175 (7) | 0.0201 (7) | 0.0274 (8) | -0.0034 (6) | -0.0032 (6) | 0.0032 (6) |
| C15B | 0.0140 (7) | 0.0156 (7) | 0.0178 (7) | 0.0017 (5) | -0.0016 (5) | -0.0006 (5) |
| C16B | 0.0156 (7) | 0.0220 (7) | 0.0179 (7) | 0.0016 (6) | -0.0007 (5) | 0.0022 (6) |
| C17B | 0.0147 (7) | 0.0229 (8) | 0.0210 (7) | -0.0005 (6) | 0.0017 (6) | -0.0001 (6) |
| C18B | 0.0123 (7) | 0.0166 (7) | 0.0207 (7) | 0.0018 (5) | -0.0012 (5) | -0.0022 (5) |
| C19B | 0.0145 (7) | 0.0189 (7) | 0.0206 (7) | 0.0025 (5) | -0.0026 (5) | 0.0040 (6) |
| C20B | 0.0129 (7) | 0.0189 (7) | 0.0216 (7) | 0.0010 (5) | -0.0005 (5) | 0.0047 (6) |

| | | | | | | |
|------|------------|-------------|-------------|-------------|-------------|-------------|
| C21B | 0.0122 (7) | 0.0181 (7) | 0.0234 (7) | 0.0003 (5) | -0.0012 (5) | -0.0022 (6) |
| C22B | 0.0136 (7) | 0.0190 (7) | 0.0237 (8) | -0.0017 (5) | -0.0006 (6) | 0.0004 (6) |
| C23B | 0.0135 (7) | 0.0173 (7) | 0.0199 (7) | 0.0007 (5) | -0.0011 (5) | -0.0032 (6) |
| C24B | 0.0166 (7) | 0.0173 (7) | 0.0198 (7) | 0.0002 (5) | -0.0004 (6) | -0.0005 (6) |
| C25B | 0.0145 (7) | 0.0173 (7) | 0.0208 (7) | -0.0012 (5) | 0.0017 (5) | -0.0033 (6) |
| C26B | 0.0113 (6) | 0.0193 (7) | 0.0203 (7) | 0.0014 (5) | -0.0008 (5) | -0.0048 (6) |
| C27B | 0.0146 (7) | 0.0178 (7) | 0.0174 (7) | 0.0038 (5) | 0.0001 (5) | -0.0009 (5) |
| C28B | 0.0123 (7) | 0.0177 (7) | 0.0233 (7) | -0.0007 (5) | 0.0009 (6) | -0.0008 (6) |
| C30B | 0.0234 (9) | 0.0391 (10) | 0.0352 (10) | 0.0069 (7) | -0.0002 (7) | 0.0114 (8) |
| C31B | 0.0262 (9) | 0.0316 (9) | 0.0275 (8) | -0.0060 (7) | 0.0061 (7) | 0.0034 (7) |
| C32B | 0.0197 (8) | 0.0351 (9) | 0.0308 (9) | 0.0056 (7) | -0.0029 (7) | 0.0111 (7) |
| C6C | 0.0117 (6) | 0.0150 (6) | 0.0200 (7) | 0.0003 (5) | 0.0005 (5) | -0.0012 (5) |
| C5C | 0.0158 (7) | 0.0133 (6) | 0.0179 (7) | -0.0030 (5) | -0.0004 (5) | 0.0002 (5) |
| C4C | 0.0097 (6) | 0.0181 (7) | 0.0222 (7) | -0.0017 (5) | -0.0010 (5) | 0.0015 (6) |
| C3C | 0.0126 (7) | 0.0165 (7) | 0.0215 (7) | 0.0018 (5) | 0.0032 (5) | 0.0014 (5) |
| C2C | 0.0132 (7) | 0.0173 (7) | 0.0181 (7) | -0.0002 (5) | -0.0001 (5) | -0.0012 (5) |
| C1C | 0.0114 (6) | 0.0145 (6) | 0.0184 (7) | -0.0008 (5) | -0.0001 (5) | 0.0009 (5) |
| C7C | 0.0101 (6) | 0.0190 (7) | 0.0192 (7) | 0.0013 (5) | -0.0001 (5) | -0.0014 (5) |
| C8C | 0.0118 (6) | 0.0170 (7) | 0.0204 (7) | 0.0011 (5) | -0.0002 (5) | -0.0014 (5) |
| C9C | 0.0122 (6) | 0.0164 (7) | 0.0152 (6) | -0.0005 (5) | -0.0019 (5) | 0.0002 (5) |
| C14C | 0.0171 (7) | 0.0277 (8) | 0.0306 (9) | 0.0085 (6) | -0.0072 (6) | -0.0138 (7) |
| C13C | 0.0189 (8) | 0.0279 (9) | 0.0336 (9) | 0.0064 (6) | -0.0112 (7) | -0.0177 (7) |
| C12C | 0.0135 (7) | 0.0162 (7) | 0.0141 (6) | -0.0011 (5) | -0.0022 (5) | -0.0005 (5) |
| C11C | 0.0112 (7) | 0.0285 (8) | 0.0233 (8) | 0.0004 (6) | 0.0012 (6) | -0.0118 (6) |
| C10C | 0.0136 (7) | 0.0261 (8) | 0.0224 (7) | -0.0021 (6) | -0.0012 (6) | -0.0121 (6) |
| C15C | 0.0124 (7) | 0.0170 (7) | 0.0152 (7) | -0.0008 (5) | -0.0025 (5) | 0.0002 (5) |
| C20C | 0.0131 (7) | 0.0304 (8) | 0.0254 (8) | 0.0002 (6) | 0.0023 (6) | -0.0146 (6) |
| C19C | 0.0131 (7) | 0.0305 (8) | 0.0260 (8) | -0.0014 (6) | -0.0014 (6) | -0.0157 (7) |
| C18C | 0.0139 (7) | 0.0166 (7) | 0.0167 (7) | -0.0010 (5) | -0.0012 (5) | -0.0009 (5) |
| C17C | 0.0162 (8) | 0.0297 (9) | 0.0366 (9) | 0.0094 (6) | -0.0095 (7) | -0.0164 (7) |
| C16C | 0.0201 (8) | 0.0278 (9) | 0.0386 (10) | 0.0064 (6) | -0.0128 (7) | -0.0198 (7) |
| C21C | 0.0123 (7) | 0.0190 (7) | 0.0190 (7) | 0.0016 (5) | -0.0011 (5) | -0.0018 (5) |
| C22C | 0.0123 (7) | 0.0183 (7) | 0.0191 (7) | 0.0003 (5) | 0.0005 (5) | -0.0027 (5) |
| C23C | 0.0116 (6) | 0.0167 (7) | 0.0156 (7) | -0.0004 (5) | -0.0006 (5) | 0.0003 (5) |
| C28C | 0.0144 (7) | 0.0148 (7) | 0.0185 (7) | 0.0010 (5) | 0.0009 (5) | -0.0014 (5) |
| C27C | 0.0158 (7) | 0.0144 (6) | 0.0172 (7) | -0.0026 (5) | -0.0010 (5) | 0.0000 (5) |
| C26C | 0.0122 (6) | 0.0165 (7) | 0.0186 (7) | -0.0010 (5) | -0.0019 (5) | 0.0015 (5) |
| C25C | 0.0126 (7) | 0.0180 (7) | 0.0177 (7) | 0.0026 (5) | 0.0015 (5) | 0.0007 (5) |
| C24C | 0.0157 (7) | 0.0175 (7) | 0.0163 (7) | 0.0003 (5) | -0.0013 (5) | -0.0039 (5) |
| C30C | 0.0208 (8) | 0.0255 (8) | 0.0283 (8) | -0.0050 (6) | -0.0059 (6) | -0.0035 (7) |
| C29C | 0.0222 (8) | 0.0270 (8) | 0.0283 (8) | 0.0052 (6) | 0.0037 (6) | -0.0075 (7) |
| C32C | 0.0295 (9) | 0.0237 (8) | 0.0303 (9) | -0.0030 (7) | 0.0044 (7) | -0.0103 (7) |
| C31C | 0.0238 (8) | 0.0255 (8) | 0.0331 (9) | 0.0055 (6) | 0.0028 (7) | -0.0094 (7) |
| O1A | 0.0116 (5) | 0.0341 (6) | 0.0274 (6) | 0.0058 (4) | 0.0015 (4) | -0.0023 (5) |
| O2A | 0.0170 (5) | 0.0343 (7) | 0.0279 (6) | -0.0068 (5) | -0.0009 (5) | -0.0123 (5) |
| O3A | 0.0144 (5) | 0.0316 (6) | 0.0292 (6) | 0.0032 (4) | -0.0014 (4) | -0.0045 (5) |
| O4A | 0.0190 (6) | 0.0215 (6) | 0.0348 (6) | -0.0035 (4) | -0.0040 (5) | -0.0049 (5) |
| O1B | 0.0161 (5) | 0.0285 (6) | 0.0319 (6) | -0.0047 (4) | 0.0011 (5) | -0.0021 (5) |

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|-----|------------|------------|------------|-------------|-------------|-------------|
| O2B | 0.0210 (6) | 0.0373 (7) | 0.0302 (6) | 0.0082 (5) | -0.0005 (5) | 0.0110 (5) |
| O3B | 0.0167 (5) | 0.0303 (6) | 0.0311 (6) | -0.0063 (5) | 0.0032 (5) | 0.0036 (5) |
| O4B | 0.0161 (5) | 0.0275 (6) | 0.0251 (6) | 0.0033 (4) | 0.0003 (4) | 0.0079 (5) |
| O2C | 0.0163 (5) | 0.0216 (5) | 0.0223 (5) | -0.0026 (4) | -0.0044 (4) | -0.0054 (4) |
| O1C | 0.0131 (5) | 0.0258 (6) | 0.0298 (6) | 0.0046 (4) | 0.0013 (4) | -0.0067 (5) |
| O4C | 0.0198 (5) | 0.0200 (5) | 0.0271 (6) | -0.0010 (4) | -0.0044 (4) | -0.0089 (4) |
| O3C | 0.0152 (5) | 0.0270 (6) | 0.0279 (6) | 0.0066 (4) | -0.0012 (4) | -0.0083 (5) |

Geometric parameters (Å, °)

| | | | |
|-----------|-------------|-----------|-------------|
| C1A—C6A | 1.387 (2) | C17B—C18B | 1.392 (2) |
| C1A—C2A | 1.401 (2) | C17B—H17B | 0.9500 |
| C1A—C7A | 1.4627 (19) | C18B—C19B | 1.398 (2) |
| C2A—C3A | 1.3817 (19) | C18B—C21B | 1.4647 (19) |
| C2A—H2A | 0.9500 | C19B—C20B | 1.3809 (19) |
| C3A—O1A | 1.3607 (18) | C19B—H19B | 0.9500 |
| C3A—C4A | 1.397 (2) | C20B—H20B | 0.9500 |
| C4A—C5A | 1.379 (2) | C21B—C22B | 1.329 (2) |
| C4A—H4A | 0.9500 | C21B—H21B | 0.9500 |
| C5A—O2A | 1.3603 (18) | C22B—C23B | 1.4650 (19) |
| C5A—C6A | 1.3933 (19) | C22B—H22B | 0.9500 |
| C6A—H6A | 0.9500 | C23B—C28B | 1.383 (2) |
| C7A—C8A | 1.333 (2) | C23B—C24B | 1.402 (2) |
| C7A—H7A | 0.9500 | C24B—C25B | 1.383 (2) |
| C8A—C9A | 1.4638 (18) | C24B—H24B | 0.9500 |
| C8A—H8A | 0.9500 | C25B—O3B | 1.3605 (18) |
| C9A—C14A | 1.391 (2) | C25B—C26B | 1.397 (2) |
| C9A—C10A | 1.398 (2) | C26B—C27B | 1.379 (2) |
| C10A—C11A | 1.3774 (19) | C26B—H26B | 0.9500 |
| C10A—H10A | 0.9500 | C27B—O4B | 1.3597 (18) |
| C11A—C12A | 1.3940 (19) | C27B—C28B | 1.3915 (19) |
| C11A—H11A | 0.9500 | C28B—H28B | 0.9500 |
| C12A—C13A | 1.392 (2) | C30B—O2B | 1.4184 (19) |
| C12A—C15A | 1.4768 (18) | C30B—H30D | 0.9800 |
| C13A—C14A | 1.3876 (19) | C30B—H30E | 0.9800 |
| C13A—H13A | 0.9500 | C30B—H30F | 0.9800 |
| C14A—H14A | 0.9500 | C31B—O3B | 1.419 (2) |
| C15A—C20A | 1.3943 (19) | C31B—H31D | 0.9800 |
| C15A—C16A | 1.396 (2) | C31B—H31E | 0.9800 |
| C16A—C17A | 1.383 (2) | C31B—H31F | 0.9800 |
| C16A—H16A | 0.9500 | C32B—O4B | 1.4224 (18) |
| C17A—C18A | 1.394 (2) | C32B—H32D | 0.9800 |
| C17A—H17A | 0.9500 | C32B—H32E | 0.9800 |
| C18A—C19A | 1.401 (2) | C32B—H32F | 0.9800 |
| C18A—C21A | 1.4654 (19) | C6C—C1C | 1.3866 (19) |
| C19A—C20A | 1.3824 (19) | C6C—C5C | 1.3957 (19) |
| C19A—H19A | 0.9500 | C6C—H6C | 0.9500 |
| C20A—H20A | 0.9500 | C5C—O2C | 1.3614 (17) |

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|-----------|-------------|-----------|-------------|
| C21A—C22A | 1.329 (2) | C5C—C4C | 1.381 (2) |
| C21A—H21A | 0.9500 | C4C—C3C | 1.397 (2) |
| C22A—C23A | 1.4649 (19) | C4C—H4C | 0.9500 |
| C22A—H22A | 0.9500 | C3C—O1C | 1.3613 (17) |
| C23A—C24A | 1.389 (2) | C3C—C2C | 1.3813 (19) |
| C23A—C28A | 1.400 (2) | C2C—C1C | 1.405 (2) |
| C24A—C25A | 1.393 (2) | C2C—H2C | 0.9500 |
| C24A—H24A | 0.9500 | C1C—C7C | 1.4651 (18) |
| C25A—O3A | 1.3559 (18) | C7C—C8C | 1.329 (2) |
| C25A—C26A | 1.381 (2) | C7C—H7C | 0.9500 |
| C26A—C27A | 1.391 (2) | C8C—C9C | 1.4637 (19) |
| C26A—H26A | 0.9500 | C8C—H8C | 0.9500 |
| C27A—O4A | 1.3615 (18) | C9C—C14C | 1.390 (2) |
| C27A—C28A | 1.3835 (19) | C9C—C10C | 1.392 (2) |
| C28A—H28A | 0.9500 | C14C—C13C | 1.382 (2) |
| C29A—O1A | 1.421 (2) | C14C—H14C | 0.9500 |
| C29A—H29A | 0.9800 | C13C—C12C | 1.392 (2) |
| C29A—H29B | 0.9800 | C13C—H13C | 0.9500 |
| C29A—H29C | 0.9800 | C12C—C11C | 1.3877 (19) |
| C30A—O2A | 1.4251 (18) | C12C—C15C | 1.4766 (19) |
| C30A—H30A | 0.9800 | C11C—C10C | 1.377 (2) |
| C30A—H30B | 0.9800 | C11C—H11C | 0.9500 |
| C30A—H30C | 0.9800 | C10C—H10C | 0.9500 |
| C31A—O3A | 1.4239 (18) | C15C—C16C | 1.389 (2) |
| C31A—H31A | 0.9800 | C15C—C20C | 1.393 (2) |
| C31A—H31B | 0.9800 | C20C—C19C | 1.377 (2) |
| C31A—H31C | 0.9800 | C20C—H20C | 0.9500 |
| C32A—O4A | 1.417 (2) | C19C—C18C | 1.393 (2) |
| C32A—H32A | 0.9800 | C19C—H19C | 0.9500 |
| C32A—H32B | 0.9800 | C18C—C17C | 1.388 (2) |
| C32A—H32C | 0.9800 | C18C—C21C | 1.4609 (19) |
| C29B—O1B | 1.4191 (18) | C17C—C16C | 1.384 (2) |
| C29B—H29D | 0.9800 | C17C—H17C | 0.9500 |
| C29B—H29E | 0.9800 | C16C—H16C | 0.9500 |
| C29B—H29F | 0.9800 | C21C—C22C | 1.327 (2) |
| C2B—C3B | 1.384 (2) | C21C—H21C | 0.9500 |
| C2B—C1B | 1.392 (2) | C22C—C23C | 1.4634 (19) |
| C2B—H2B | 0.9500 | C22C—H22C | 0.9500 |
| C3B—O1B | 1.3608 (19) | C23C—C28C | 1.3906 (19) |
| C3B—C4B | 1.399 (2) | C23C—C24C | 1.395 (2) |
| C4B—C5B | 1.382 (2) | C28C—C27C | 1.3892 (19) |
| C4B—H4B | 0.9500 | C28C—H28C | 0.9500 |
| C5B—O2B | 1.3719 (19) | C27C—O4C | 1.3607 (17) |
| C5B—C6B | 1.385 (2) | C27C—C26C | 1.383 (2) |
| C6B—C1B | 1.394 (2) | C26C—C25C | 1.387 (2) |
| C6B—H6B | 0.9500 | C26C—H26C | 0.9500 |
| C1B—C7B | 1.4638 (19) | C25C—O3C | 1.3602 (17) |
| C7B—C8B | 1.334 (2) | C25C—C24C | 1.3880 (19) |

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| C7B—H7B | 0.9500 | C24C—H24C | 0.9500 |
| C8B—C9B | 1.464 (2) | C30C—O2C | 1.4259 (17) |
| C8B—H8B | 0.9500 | C30C—H30G | 0.9800 |
| C9B—C14B | 1.394 (2) | C30C—H30H | 0.9800 |
| C9B—C10B | 1.400 (2) | C30C—H30I | 0.9800 |
| C10B—C11B | 1.3825 (19) | C29C—O1C | 1.4274 (19) |
| C10B—H10B | 0.9500 | C29C—H29G | 0.9800 |
| C11B—C12B | 1.3980 (19) | C29C—H29H | 0.9800 |
| C11B—H11B | 0.9500 | C29C—H29I | 0.9800 |
| C12B—C13B | 1.397 (2) | C32C—O4C | 1.4278 (19) |
| C12B—C15B | 1.4760 (19) | C32C—H32G | 0.9800 |
| C13B—C14B | 1.384 (2) | C32C—H32H | 0.9800 |
| C13B—H13B | 0.9500 | C32C—H32I | 0.9800 |
| C14B—H14B | 0.9500 | C31C—O3C | 1.4191 (19) |
| C15B—C16B | 1.393 (2) | C31C—H31G | 0.9800 |
| C15B—C20B | 1.395 (2) | C31C—H31H | 0.9800 |
| C16B—C17B | 1.3861 (19) | C31C—H31I | 0.9800 |
| C16B—H16B | 0.9500 | | |
| | | | |
| C6A—C1A—C2A | 119.76 (13) | C20B—C19B—C18B | 121.23 (14) |
| C6A—C1A—C7A | 117.44 (13) | C20B—C19B—H19B | 119.4 |
| C2A—C1A—C7A | 122.80 (13) | C18B—C19B—H19B | 119.4 |
| C3A—C2A—C1A | 119.03 (13) | C19B—C20B—C15B | 121.26 (14) |
| C3A—C2A—H2A | 120.5 | C19B—C20B—H20B | 119.4 |
| C1A—C2A—H2A | 120.5 | C15B—C20B—H20B | 119.4 |
| O1A—C3A—C2A | 124.27 (14) | C22B—C21B—C18B | 125.08 (14) |
| O1A—C3A—C4A | 114.28 (13) | C22B—C21B—H21B | 117.5 |
| C2A—C3A—C4A | 121.45 (14) | C18B—C21B—H21B | 117.5 |
| C5A—C4A—C3A | 119.08 (13) | C21B—C22B—C23B | 127.82 (14) |
| C5A—C4A—H4A | 120.5 | C21B—C22B—H22B | 116.1 |
| C3A—C4A—H4A | 120.5 | C23B—C22B—H22B | 116.1 |
| O2A—C5A—C4A | 124.70 (13) | C28B—C23B—C24B | 119.66 (13) |
| O2A—C5A—C6A | 115.09 (13) | C28B—C23B—C22B | 117.36 (13) |
| C4A—C5A—C6A | 120.21 (14) | C24B—C23B—C22B | 122.98 (13) |
| C1A—C6A—C5A | 120.46 (14) | C25B—C24B—C23B | 119.19 (14) |
| C1A—C6A—H6A | 119.8 | C25B—C24B—H24B | 120.4 |
| C5A—C6A—H6A | 119.8 | C23B—C24B—H24B | 120.4 |
| C8A—C7A—C1A | 128.11 (14) | O3B—C25B—C24B | 124.61 (14) |
| C8A—C7A—H7A | 115.9 | O3B—C25B—C26B | 114.15 (13) |
| C1A—C7A—H7A | 115.9 | C24B—C25B—C26B | 121.24 (13) |
| C7A—C8A—C9A | 124.89 (13) | C27B—C26B—C25B | 118.99 (13) |
| C7A—C8A—H8A | 117.6 | C27B—C26B—H26B | 120.5 |
| C9A—C8A—H8A | 117.6 | C25B—C26B—H26B | 120.5 |
| C14A—C9A—C10A | 117.26 (13) | O4B—C27B—C26B | 124.28 (13) |
| C14A—C9A—C8A | 120.30 (13) | O4B—C27B—C28B | 115.31 (13) |
| C10A—C9A—C8A | 122.44 (13) | C26B—C27B—C28B | 120.41 (13) |
| C11A—C10A—C9A | 121.14 (13) | C23B—C28B—C27B | 120.48 (14) |
| C11A—C10A—H10A | 119.4 | C23B—C28B—H28B | 119.8 |

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| C9A—C10A—H10A | 119.4 | C27B—C28B—H28B | 119.8 |
| C10A—C11A—C12A | 121.61 (14) | O2B—C30B—H30D | 109.5 |
| C10A—C11A—H11A | 119.2 | O2B—C30B—H30E | 109.5 |
| C12A—C11A—H11A | 119.2 | H30D—C30B—H30E | 109.5 |
| C13A—C12A—C11A | 117.47 (13) | O2B—C30B—H30F | 109.5 |
| C13A—C12A—C15A | 122.48 (13) | H30D—C30B—H30F | 109.5 |
| C11A—C12A—C15A | 120.05 (13) | H30E—C30B—H30F | 109.5 |
| C14A—C13A—C12A | 120.88 (13) | O3B—C31B—H31D | 109.5 |
| C14A—C13A—H13A | 119.6 | O3B—C31B—H31E | 109.5 |
| C12A—C13A—H13A | 119.6 | H31D—C31B—H31E | 109.5 |
| C13A—C14A—C9A | 121.62 (13) | O3B—C31B—H31F | 109.5 |
| C13A—C14A—H14A | 119.2 | H31D—C31B—H31F | 109.5 |
| C9A—C14A—H14A | 119.2 | H31E—C31B—H31F | 109.5 |
| C20A—C15A—C16A | 117.33 (13) | O4B—C32B—H32D | 109.5 |
| C20A—C15A—C12A | 121.80 (13) | O4B—C32B—H32E | 109.5 |
| C16A—C15A—C12A | 120.84 (13) | H32D—C32B—H32E | 109.5 |
| C17A—C16A—C15A | 121.45 (14) | O4B—C32B—H32F | 109.5 |
| C17A—C16A—H16A | 119.3 | H32D—C32B—H32F | 109.5 |
| C15A—C16A—H16A | 119.3 | H32E—C32B—H32F | 109.5 |
| C16A—C17A—C18A | 121.20 (14) | C1C—C6C—C5C | 120.45 (13) |
| C16A—C17A—H17A | 119.4 | C1C—C6C—H6C | 119.8 |
| C18A—C17A—H17A | 119.4 | C5C—C6C—H6C | 119.8 |
| C17A—C18A—C19A | 117.48 (13) | O2C—C5C—C4C | 124.48 (13) |
| C17A—C18A—C21A | 119.24 (14) | O2C—C5C—C6C | 115.20 (13) |
| C19A—C18A—C21A | 123.25 (13) | C4C—C5C—C6C | 120.31 (13) |
| C20A—C19A—C18A | 121.08 (13) | C5C—C4C—C3C | 118.99 (13) |
| C20A—C19A—H19A | 119.5 | C5C—C4C—H4C | 120.5 |
| C18A—C19A—H19A | 119.5 | C3C—C4C—H4C | 120.5 |
| C19A—C20A—C15A | 121.44 (13) | O1C—C3C—C2C | 124.23 (13) |
| C19A—C20A—H20A | 119.3 | O1C—C3C—C4C | 114.29 (12) |
| C15A—C20A—H20A | 119.3 | C2C—C3C—C4C | 121.47 (13) |
| C22A—C21A—C18A | 126.04 (14) | C3C—C2C—C1C | 119.16 (13) |
| C22A—C21A—H21A | 117.0 | C3C—C2C—H2C | 120.4 |
| C18A—C21A—H21A | 117.0 | C1C—C2C—H2C | 120.4 |
| C21A—C22A—C23A | 127.20 (14) | C6C—C1C—C2C | 119.61 (13) |
| C21A—C22A—H22A | 116.4 | C6C—C1C—C7C | 118.07 (13) |
| C23A—C22A—H22A | 116.4 | C2C—C1C—C7C | 122.31 (13) |
| C24A—C23A—C28A | 119.52 (13) | C8C—C7C—C1C | 127.38 (13) |
| C24A—C23A—C22A | 123.22 (13) | C8C—C7C—H7C | 116.3 |
| C28A—C23A—C22A | 117.26 (13) | C1C—C7C—H7C | 116.3 |
| C23A—C24A—C25A | 119.94 (14) | C7C—C8C—C9C | 125.69 (13) |
| C23A—C24A—H24A | 120.0 | C7C—C8C—H8C | 117.2 |
| C25A—C24A—H24A | 120.0 | C9C—C8C—H8C | 117.2 |
| O3A—C25A—C26A | 123.32 (13) | C14C—C9C—C10C | 116.93 (13) |
| O3A—C25A—C24A | 115.83 (13) | C14C—C9C—C8C | 119.64 (13) |
| C26A—C25A—C24A | 120.84 (14) | C10C—C9C—C8C | 123.42 (13) |
| C25A—C26A—C27A | 118.96 (13) | C13C—C14C—C9C | 121.58 (14) |
| C25A—C26A—H26A | 120.5 | C13C—C14C—H14C | 119.2 |

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| C27A—C26A—H26A | 120.5 | C9C—C14C—H14C | 119.2 |
| O4A—C27A—C28A | 124.38 (14) | C14C—C13C—C12C | 121.57 (14) |
| O4A—C27A—C26A | 114.51 (13) | C14C—C13C—H13C | 119.2 |
| C28A—C27A—C26A | 121.11 (14) | C12C—C13C—H13C | 119.2 |
| C27A—C28A—C23A | 119.63 (14) | C11C—C12C—C13C | 116.48 (13) |
| C27A—C28A—H28A | 120.2 | C11C—C12C—C15C | 121.35 (13) |
| C23A—C28A—H28A | 120.2 | C13C—C12C—C15C | 122.17 (13) |
| O1A—C29A—H29A | 109.5 | C10C—C11C—C12C | 122.23 (14) |
| O1A—C29A—H29B | 109.5 | C10C—C11C—H11C | 118.9 |
| H29A—C29A—H29B | 109.5 | C12C—C11C—H11C | 118.9 |
| O1A—C29A—H29C | 109.5 | C11C—C10C—C9C | 121.22 (13) |
| H29A—C29A—H29C | 109.5 | C11C—C10C—H10C | 119.4 |
| H29B—C29A—H29C | 109.5 | C9C—C10C—H10C | 119.4 |
| O2A—C30A—H30A | 109.5 | C16C—C15C—C20C | 116.37 (13) |
| O2A—C30A—H30B | 109.5 | C16C—C15C—C12C | 122.08 (13) |
| H30A—C30A—H30B | 109.5 | C20C—C15C—C12C | 121.52 (13) |
| O2A—C30A—H30C | 109.5 | C19C—C20C—C15C | 122.10 (14) |
| H30A—C30A—H30C | 109.5 | C19C—C20C—H20C | 118.9 |
| H30B—C30A—H30C | 109.5 | C15C—C20C—H20C | 118.9 |
| O3A—C31A—H31A | 109.5 | C20C—C19C—C18C | 121.35 (14) |
| O3A—C31A—H31B | 109.5 | C20C—C19C—H19C | 119.3 |
| H31A—C31A—H31B | 109.5 | C18C—C19C—H19C | 119.3 |
| O3A—C31A—H31C | 109.5 | C17C—C18C—C19C | 116.81 (13) |
| H31A—C31A—H31C | 109.5 | C17C—C18C—C21C | 120.05 (13) |
| H31B—C31A—H31C | 109.5 | C19C—C18C—C21C | 123.15 (13) |
| O4A—C32A—H32A | 109.5 | C16C—C17C—C18C | 121.65 (15) |
| O4A—C32A—H32B | 109.5 | C16C—C17C—H17C | 119.2 |
| H32A—C32A—H32B | 109.5 | C18C—C17C—H17C | 119.2 |
| O4A—C32A—H32C | 109.5 | C17C—C16C—C15C | 121.70 (14) |
| H32A—C32A—H32C | 109.5 | C17C—C16C—H16C | 119.1 |
| H32B—C32A—H32C | 109.5 | C15C—C16C—H16C | 119.1 |
| O1B—C29B—H29D | 109.5 | C22C—C21C—C18C | 125.94 (14) |
| O1B—C29B—H29E | 109.5 | C22C—C21C—H21C | 117.0 |
| H29D—C29B—H29E | 109.5 | C18C—C21C—H21C | 117.0 |
| O1B—C29B—H29F | 109.5 | C21C—C22C—C23C | 127.19 (14) |
| H29D—C29B—H29F | 109.5 | C21C—C22C—H22C | 116.4 |
| H29E—C29B—H29F | 109.5 | C23C—C22C—H22C | 116.4 |
| C3B—C2B—C1B | 119.53 (14) | C28C—C23C—C24C | 119.95 (13) |
| C3B—C2B—H2B | 120.2 | C28C—C23C—C22C | 117.63 (13) |
| C1B—C2B—H2B | 120.2 | C24C—C23C—C22C | 122.43 (13) |
| O1B—C3B—C2B | 115.13 (14) | C27C—C28C—C23C | 119.94 (13) |
| O1B—C3B—C4B | 123.32 (13) | C27C—C28C—H28C | 120.0 |
| C2B—C3B—C4B | 121.56 (14) | C23C—C28C—H28C | 120.0 |
| C5B—C4B—C3B | 118.33 (13) | O4C—C27C—C26C | 115.61 (12) |
| C5B—C4B—H4B | 120.8 | O4C—C27C—C28C | 123.97 (13) |
| C3B—C4B—H4B | 120.8 | C26C—C27C—C28C | 120.41 (13) |
| O2B—C5B—C4B | 124.50 (14) | C27C—C26C—C25C | 119.49 (13) |
| O2B—C5B—C6B | 114.80 (14) | C27C—C26C—H26C | 120.3 |

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| C4B—C5B—C6B | 120.71 (14) | C25C—C26C—H26C | 120.3 |
| C5B—C6B—C1B | 120.73 (14) | O3C—C25C—C26C | 115.12 (12) |
| C5B—C6B—H6B | 119.6 | O3C—C25C—C24C | 123.99 (13) |
| C1B—C6B—H6B | 119.6 | C26C—C25C—C24C | 120.89 (13) |
| C2B—C1B—C6B | 119.13 (13) | C25C—C24C—C23C | 119.31 (13) |
| C2B—C1B—C7B | 123.39 (14) | C25C—C24C—H24C | 120.3 |
| C6B—C1B—C7B | 117.48 (14) | C23C—C24C—H24C | 120.3 |
| C8B—C7B—C1B | 128.17 (14) | O2C—C30C—H30G | 109.5 |
| C8B—C7B—H7B | 115.9 | O2C—C30C—H30H | 109.5 |
| C1B—C7B—H7B | 115.9 | H30G—C30C—H30H | 109.5 |
| C7B—C8B—C9B | 125.49 (14) | O2C—C30C—H30I | 109.5 |
| C7B—C8B—H8B | 117.3 | H30G—C30C—H30I | 109.5 |
| C9B—C8B—H8B | 117.3 | H30H—C30C—H30I | 109.5 |
| C14B—C9B—C10B | 117.48 (13) | O1C—C29C—H29G | 109.5 |
| C14B—C9B—C8B | 119.89 (13) | O1C—C29C—H29H | 109.5 |
| C10B—C9B—C8B | 122.63 (13) | H29G—C29C—H29H | 109.5 |
| C11B—C10B—C9B | 121.01 (13) | O1C—C29C—H29I | 109.5 |
| C11B—C10B—H10B | 119.5 | H29G—C29C—H29I | 109.5 |
| C9B—C10B—H10B | 119.5 | H29H—C29C—H29I | 109.5 |
| C10B—C11B—C12B | 121.56 (13) | O4C—C32C—H32G | 109.5 |
| C10B—C11B—H11B | 119.2 | O4C—C32C—H32H | 109.5 |
| C12B—C11B—H11B | 119.2 | H32G—C32C—H32H | 109.5 |
| C13B—C12B—C11B | 117.30 (13) | O4C—C32C—H32I | 109.5 |
| C13B—C12B—C15B | 121.30 (13) | H32G—C32C—H32I | 109.5 |
| C11B—C12B—C15B | 121.40 (13) | H32H—C32C—H32I | 109.5 |
| C14B—C13B—C12B | 121.20 (14) | O3C—C31C—H31G | 109.5 |
| C14B—C13B—H13B | 119.4 | O3C—C31C—H31H | 109.5 |
| C12B—C13B—H13B | 119.4 | H31G—C31C—H31H | 109.5 |
| C13B—C14B—C9B | 121.44 (14) | O3C—C31C—H31I | 109.5 |
| C13B—C14B—H14B | 119.3 | H31G—C31C—H31I | 109.5 |
| C9B—C14B—H14B | 119.3 | H31H—C31C—H31I | 109.5 |
| C16B—C15B—C20B | 117.71 (13) | C3A—O1A—C29A | 116.65 (12) |
| C16B—C15B—C12B | 121.83 (13) | C5A—O2A—C30A | 117.18 (13) |
| C20B—C15B—C12B | 120.47 (13) | C25A—O3A—C31A | 118.07 (12) |
| C17B—C16B—C15B | 120.92 (14) | C27A—O4A—C32A | 117.23 (12) |
| C17B—C16B—H16B | 119.5 | C3B—O1B—C29B | 118.41 (13) |
| C15B—C16B—H16B | 119.5 | C5B—O2B—C30B | 117.89 (13) |
| C16B—C17B—C18B | 121.51 (14) | C25B—O3B—C31B | 116.87 (12) |
| C16B—C17B—H17B | 119.2 | C27B—O4B—C32B | 116.82 (12) |
| C18B—C17B—H17B | 119.2 | C5C—O2C—C30C | 117.52 (12) |
| C17B—C18B—C19B | 117.37 (13) | C3C—O1C—C29C | 117.02 (12) |
| C17B—C18B—C21B | 119.56 (13) | C27C—O4C—C32C | 117.52 (12) |
| C19B—C18B—C21B | 123.07 (13) | C25C—O3C—C31C | 117.45 (12) |
| C6A—C1A—C2A—C3A | -0.5 (2) | C17B—C18B—C21B—C22B | 177.60 (15) |
| C7A—C1A—C2A—C3A | 179.58 (14) | C19B—C18B—C21B—C22B | -2.8 (2) |
| C1A—C2A—C3A—O1A | 179.44 (14) | C18B—C21B—C22B—C23B | 179.20 (14) |
| C1A—C2A—C3A—C4A | 0.0 (2) | C21B—C22B—C23B—C28B | 175.56 (15) |

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| O1A—C3A—C4A—C5A | -178.75 (13) | C21B—C22B—C23B—C24B | -4.5 (2) |
| C2A—C3A—C4A—C5A | 0.8 (2) | C28B—C23B—C24B—C25B | 1.6 (2) |
| C3A—C4A—C5A—O2A | 179.50 (14) | C22B—C23B—C24B—C25B | -178.41 (13) |
| C3A—C4A—C5A—C6A | -0.9 (2) | C23B—C24B—C25B—O3B | 179.65 (14) |
| C2A—C1A—C6A—C5A | 0.4 (2) | C23B—C24B—C25B—C26B | -0.7 (2) |
| C7A—C1A—C6A—C5A | -179.74 (13) | O3B—C25B—C26B—C27B | 178.71 (13) |
| O2A—C5A—C6A—C1A | 179.98 (14) | C24B—C25B—C26B—C27B | -1.0 (2) |
| C4A—C5A—C6A—C1A | 0.4 (2) | C25B—C26B—C27B—O4B | -178.84 (13) |
| C6A—C1A—C7A—C8A | -173.06 (16) | C25B—C26B—C27B—C28B | 1.8 (2) |
| C2A—C1A—C7A—C8A | 6.8 (2) | C24B—C23B—C28B—C27B | -0.8 (2) |
| C1A—C7A—C8A—C9A | -179.23 (14) | C22B—C23B—C28B—C27B | 179.17 (13) |
| C7A—C8A—C9A—C14A | 179.00 (15) | O4B—C27B—C28B—C23B | 179.68 (13) |
| C7A—C8A—C9A—C10A | -0.4 (2) | C26B—C27B—C28B—C23B | -0.9 (2) |
| C14A—C9A—C10A—C11A | 0.5 (2) | C1C—C6C—C5C—O2C | -178.51 (13) |
| C8A—C9A—C10A—C11A | 179.95 (14) | C1C—C6C—C5C—C4C | 0.5 (2) |
| C9A—C10A—C11A—C12A | 0.2 (2) | O2C—C5C—C4C—C3C | 178.37 (13) |
| C10A—C11A—C12A—C13A | -1.0 (2) | C6C—C5C—C4C—C3C | -0.5 (2) |
| C10A—C11A—C12A—C15A | 179.27 (14) | C5C—C4C—C3C—O1C | -179.65 (13) |
| C11A—C12A—C13A—C14A | 1.1 (2) | C5C—C4C—C3C—C2C | 0.3 (2) |
| C15A—C12A—C13A—C14A | -179.21 (13) | O1C—C3C—C2C—C1C | 179.92 (14) |
| C12A—C13A—C14A—C9A | -0.4 (2) | C4C—C3C—C2C—C1C | 0.0 (2) |
| C10A—C9A—C14A—C13A | -0.4 (2) | C5C—C6C—C1C—C2C | -0.2 (2) |
| C8A—C9A—C14A—C13A | -179.89 (13) | C5C—C6C—C1C—C7C | 179.33 (13) |
| C13A—C12A—C15A—C20A | -31.9 (2) | C3C—C2C—C1C—C6C | 0.0 (2) |
| C11A—C12A—C15A—C20A | 147.87 (15) | C3C—C2C—C1C—C7C | -179.55 (13) |
| C13A—C12A—C15A—C16A | 150.00 (15) | C6C—C1C—C7C—C8C | 178.32 (15) |
| C11A—C12A—C15A—C16A | -30.3 (2) | C2C—C1C—C7C—C8C | -2.2 (2) |
| C20A—C15A—C16A—C17A | -1.5 (2) | C1C—C7C—C8C—C9C | 178.72 (14) |
| C12A—C15A—C16A—C17A | 176.78 (15) | C7C—C8C—C9C—C14C | -170.93 (16) |
| C15A—C16A—C17A—C18A | 0.9 (3) | C7C—C8C—C9C—C10C | 7.9 (2) |
| C16A—C17A—C18A—C19A | 0.3 (2) | C10C—C9C—C14C—C13C | -0.4 (3) |
| C16A—C17A—C18A—C21A | 178.35 (15) | C8C—C9C—C14C—C13C | 178.54 (16) |
| C17A—C18A—C19A—C20A | -0.7 (2) | C9C—C14C—C13C—C12C | 0.7 (3) |
| C21A—C18A—C19A—C20A | -178.74 (14) | C14C—C13C—C12C—C11C | -0.7 (3) |
| C18A—C19A—C20A—C15A | 0.1 (2) | C14C—C13C—C12C—C15C | 178.57 (16) |
| C16A—C15A—C20A—C19A | 1.0 (2) | C13C—C12C—C11C—C10C | 0.4 (2) |
| C12A—C15A—C20A—C19A | -177.24 (13) | C15C—C12C—C11C—C10C | -178.83 (15) |
| C17A—C18A—C21A—C22A | -166.43 (16) | C12C—C11C—C10C—C9C | -0.2 (3) |
| C19A—C18A—C21A—C22A | 11.5 (2) | C14C—C9C—C10C—C11C | 0.1 (2) |
| C18A—C21A—C22A—C23A | 178.86 (14) | C8C—C9C—C10C—C11C | -178.75 (15) |
| C21A—C22A—C23A—C24A | -3.0 (2) | C11C—C12C—C15C—C16C | 2.9 (2) |
| C21A—C22A—C23A—C28A | 176.53 (15) | C13C—C12C—C15C—C16C | -176.30 (16) |
| C28A—C23A—C24A—C25A | -0.5 (2) | C11C—C12C—C15C—C20C | -175.23 (15) |
| C22A—C23A—C24A—C25A | 179.02 (13) | C13C—C12C—C15C—C20C | 5.5 (2) |
| C23A—C24A—C25A—O3A | 179.81 (13) | C16C—C15C—C20C—C19C | -0.4 (2) |
| C23A—C24A—C25A—C26A | 0.2 (2) | C12C—C15C—C20C—C19C | 177.83 (15) |
| O3A—C25A—C26A—C27A | -179.18 (13) | C15C—C20C—C19C—C18C | 0.0 (3) |
| C24A—C25A—C26A—C27A | 0.5 (2) | C20C—C19C—C18C—C17C | -0.3 (3) |

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| C25A—C26A—C27A—O4A | -179.96 (13) | C20C—C19C—C18C—C21C | 179.99 (15) |
| C25A—C26A—C27A—C28A | -0.7 (2) | C19C—C18C—C17C—C16C | 1.1 (3) |
| O4A—C27A—C28A—C23A | 179.51 (13) | C21C—C18C—C17C—C16C | -179.18 (16) |
| C26A—C27A—C28A—C23A | 0.3 (2) | C18C—C17C—C16C—C15C | -1.6 (3) |
| C24A—C23A—C28A—C27A | 0.3 (2) | C20C—C15C—C16C—C17C | 1.2 (3) |
| C22A—C23A—C28A—C27A | -179.27 (13) | C12C—C15C—C16C—C17C | -177.03 (16) |
| C1B—C2B—C3B—O1B | -179.80 (13) | C17C—C18C—C21C—C22C | 168.93 (16) |
| C1B—C2B—C3B—C4B | -0.1 (2) | C19C—C18C—C21C—C22C | -11.3 (2) |
| O1B—C3B—C4B—C5B | 179.74 (14) | C18C—C21C—C22C—C23C | 179.92 (14) |
| C2B—C3B—C4B—C5B | 0.1 (2) | C21C—C22C—C23C—C28C | -171.75 (15) |
| C3B—C4B—C5B—O2B | -179.20 (14) | C21C—C22C—C23C—C24C | 8.0 (2) |
| C3B—C4B—C5B—C6B | 0.5 (2) | C24C—C23C—C28C—C27C | -0.2 (2) |
| O2B—C5B—C6B—C1B | 178.66 (14) | C22C—C23C—C28C—C27C | 179.64 (13) |
| C4B—C5B—C6B—C1B | -1.1 (2) | C23C—C28C—C27C—O4C | -179.64 (13) |
| C3B—C2B—C1B—C6B | -0.4 (2) | C23C—C28C—C27C—C26C | 0.1 (2) |
| C3B—C2B—C1B—C7B | -179.55 (13) | O4C—C27C—C26C—C25C | 179.99 (13) |
| C5B—C6B—C1B—C2B | 1.0 (2) | C28C—C27C—C26C—C25C | 0.3 (2) |
| C5B—C6B—C1B—C7B | -179.80 (13) | C27C—C26C—C25C—O3C | 179.86 (13) |
| C2B—C1B—C7B—C8B | -2.4 (2) | C27C—C26C—C25C—C24C | -0.5 (2) |
| C6B—C1B—C7B—C8B | 178.46 (15) | O3C—C25C—C24C—C23C | -179.99 (14) |
| C1B—C7B—C8B—C9B | 179.96 (14) | C26C—C25C—C24C—C23C | 0.4 (2) |
| C7B—C8B—C9B—C14B | 168.33 (16) | C28C—C23C—C24C—C25C | -0.1 (2) |
| C7B—C8B—C9B—C10B | -11.0 (2) | C22C—C23C—C24C—C25C | -179.86 (13) |
| C14B—C9B—C10B—C11B | 0.8 (2) | C2A—C3A—O1A—C29A | 7.8 (2) |
| C8B—C9B—C10B—C11B | -179.79 (14) | C4A—C3A—O1A—C29A | -172.69 (14) |
| C9B—C10B—C11B—C12B | -0.2 (2) | C4A—C5A—O2A—C30A | -10.2 (2) |
| C10B—C11B—C12B—C13B | -0.8 (2) | C6A—C5A—O2A—C30A | 170.20 (15) |
| C10B—C11B—C12B—C15B | 178.33 (13) | C26A—C25A—O3A—C31A | -3.1 (2) |
| C11B—C12B—C13B—C14B | 1.3 (2) | C24A—C25A—O3A—C31A | 177.21 (14) |
| C15B—C12B—C13B—C14B | -177.88 (14) | C28A—C27A—O4A—C32A | 5.3 (2) |
| C12B—C13B—C14B—C9B | -0.7 (2) | C26A—C27A—O4A—C32A | -175.46 (14) |
| C10B—C9B—C14B—C13B | -0.4 (2) | C2B—C3B—O1B—C29B | -173.65 (13) |
| C8B—C9B—C14B—C13B | -179.78 (15) | C4B—C3B—O1B—C29B | 6.7 (2) |
| C13B—C12B—C15B—C16B | -149.58 (15) | C4B—C5B—O2B—C30B | -8.0 (2) |
| C11B—C12B—C15B—C16B | 31.3 (2) | C6B—C5B—O2B—C30B | 172.27 (15) |
| C13B—C12B—C15B—C20B | 29.9 (2) | C24B—C25B—O3B—C31B | -7.4 (2) |
| C11B—C12B—C15B—C20B | -149.26 (14) | C26B—C25B—O3B—C31B | 172.87 (13) |
| C20B—C15B—C16B—C17B | -0.9 (2) | C26B—C27B—O4B—C32B | 10.7 (2) |
| C12B—C15B—C16B—C17B | 178.55 (13) | C28B—C27B—O4B—C32B | -169.93 (14) |
| C15B—C16B—C17B—C18B | 0.4 (2) | C4C—C5C—O2C—C30C | 5.9 (2) |
| C16B—C17B—C18B—C19B | 0.4 (2) | C6C—C5C—O2C—C30C | -175.15 (13) |
| C16B—C17B—C18B—C21B | -179.96 (14) | C2C—C3C—O1C—C29C | -12.6 (2) |
| C17B—C18B—C19B—C20B | -0.7 (2) | C4C—C3C—O1C—C29C | 167.30 (13) |
| C21B—C18B—C19B—C20B | 179.72 (14) | C26C—C27C—O4C—C32C | 172.34 (14) |
| C18B—C19B—C20B—C15B | 0.1 (2) | C28C—C27C—O4C—C32C | -7.9 (2) |
| C16B—C15B—C20B—C19B | 0.7 (2) | C26C—C25C—O3C—C31C | -170.26 (14) |
| C12B—C15B—C20B—C19B | -178.81 (14) | C24C—C25C—O3C—C31C | 10.1 (2) |
