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# Tris(2,6-dibenzoyl-4-methylphenolato-$\kappa^2O^1,O^2$)cobalt(III)

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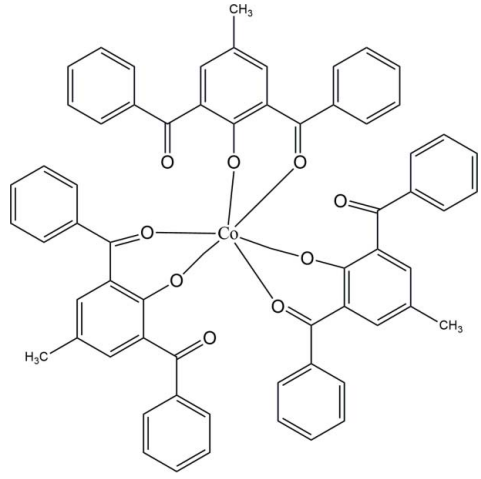
Key indicators: single-crystal X-ray study; $T$ = 123 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.055; $wR$ factor = 0.154; data-to-parameter ratio = 15.3.

In the title compound, $[Co(C_{21}H_{15}O_3)_3]$, the $Co^{III}$ ion is coordinated in a slightly distorted octahedral environment by three phenolate O and three benzoyl O atoms from three monoanionic bidentate 2,6-dibenzoyl-4-methylphenolate ligands. The dihedral angles between the mean planes of the central phenolate rings and the peripheral phenyl rings are 46.62 (10)/87.06 (9), 60.44 (8)/23.13 (8) and 46.49 (6)/65.29 (6)°. The crystal packing is stabilized by weak intermolecular C—H···O interactions. Molecules are further linked by two $\pi$–$\pi$ [centroid–centroid distances = 3.8612 (14) and 3.9479 (14) Å] and four C—H···$\pi$ interactions, forming a three-dimensional network.

## Related literature

For phenol-based diketones, see: Gupta *et al.* (2002, 2012*a*). For material and biological applications, see: Church & Halvorson (1959); Olsson *et al.* (2005); Burschka *et al.* (2013); Erkkila *et al.* (1999); Metcalfe & Thomas (2003); Generex & Barton (2010). For related structures, see: Gupta *et al.* (2012*b*); Huang *et al.* (2013).




## Experimental

### Crystal data

$[Co(C_{21}H_{15}O_3)_3]$
$M_r$ = 1004.92
Monoclinic, $P2_1/c$
$a$ = 11.2858 (3) Å
$b$ = 17.5442 (4) Å
$c$ = 24.7745 (5) Å
$\beta$ = 92.8922 (19)°
$V$ = 4899.12 (19) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 3.25 mm$^{-1}$
$T$ = 123 K
0.46 × 0.18 × 0.15 mm

### Data collection

Agilent Xcalibur (Ruby, Gemini) diffractometer
Absorption correction: analytical [*CrysAlis PRO* (Agilent, 2012), based on expressions derived by Clark & Reid (1995)]
$T_{min}$ = 0.477, $T_{max}$ = 0.705
21885 measured reflections
10145 independent reflections
9001 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.045

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.154
$S$ = 1.06
10145 reflections
661 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.62 e Å$^{-3}$

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

*Cg*7, *Cg*9, *Cg*11 and *Cg*12 are the centroids of the C9*A*–C14*A*, C9*C*–C14*C*, C16*B*–C21*B* and C16*C*–C21*C* rings, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C12*A*—H12*A*···O2*B*$^{i}$ | 0.95 | 2.60 | 3.442 (3) | 147 |
| C13*A*—H13*A*···O3*C*$^{i}$ | 0.95 | 2.48 | 3.278 (3) | 141 |
| C13*B*—H13*B*···O3*B*$^{ii}$ | 0.95 | 2.39 | 3.311 (3) | 162 |
| C11*C*—H11*C*···O3*C*$^{iii}$ | 0.95 | 2.40 | 3.313 (3) | 161 |
| C10*B*—H10*B*···*Cg*12 | 0.95 | 2.70 | 3.634 (3) | 166 |
| C11*B*—H11*B*···*Cg*7$^{iv}$ | 0.95 | 2.72 | 3.479 (3) | 137 |
| C18*C*—H18*C*···*Cg*9$^{iv}$ | 0.95 | 2.99 | 3.720 (4) | 135 |
| C20*C*—H20*C*···*Cg*11$^{v}$ | 0.95 | 2.88 | 3.332 (3) | 110 |

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x+1, y, z$; (v) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics:

*SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HG5379).

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# supplementary materials

*Acta Cryst.* (2014). E**70**, m67–m68 [doi:10.1107/S1600536814001664]

## Tris(2,6-dibenzoyl-4-methylphenolato-$\kappa^2O^1,O^2$)cobalt(III)

**Abhishek K. Gupta, Sanjay Srivastava and Ray J. Butcher**

### 1. Comment

In recent years phenol-based diketones have been widely used as ligands forming complexes with interesting properties that are useful in material science (Church & Halvorson, 1959; Olsson *et al.*, 2005; Burschka *et al.*, 2013) and in biological systems (Erkkila *et al.*, 1999; Metcalfe & Thomas, 2003; Generex & Barton, 2010). The crystal structure of 4-methyl-2,6-dibenzoylphenol (mdbpH)), 4-*tert*-butyl-2,6-dibenzoylphenol (bdbpH) and their chromium(III) complexes have been reported earlier (Gupta *et al.*, 2002, 2012*a*, 2012*b*). We herein report the synthesis and X-ray crystal structure analysis of the title compound.

The molecular structure of the title compound, $[Co(C_{21}H_{15}O_3)_3]$, is shown in (Fig.1). The three monoanionic ligands $(2,6\text{-}PhCO)_2(4\text{-}Me)C_6H_2O^-$ are bidentate, coordinating through phenolic O and benzoyl O atoms to give a *mer*–$CoO_3O_3$ octahedral configuration. The coordination geometry around the Co(III) ion deviates slightly from an ideal octahedral coordination as evidenced by the *trans* angles, O1C/Co/O1A (178.32 (7)°), O2B/Co/O2C (176.88 (7)°) and O1B/Co/O2A (178.76 (7)°). The remaining angles vary between 87.01 (7)° and 93.25 (7)°, whereby the smallest values correspond to the O–Co–O bond angles in the three chelate rings, O1A/Co/O2A 88.47 (7)°, O1B/Co/O2B 90.02 (7)° and O1C/Co/O2C 87.01 (7)°. The Co–O (phenolic) distances [mean 1.932 Å] are similar and comparable to those reported for other mononuclear complexes, [Cr(mdbp)$_3$, mean 1.931 Å] (Gupta *et al.*, 2012*b*) and [Co$L_3$] (*L* = 4- bromo-2-(methylimino-methyl)phenolate) [mean 1.890 Å] (Huang *et al.*, 2013) but significantly shorter than the Co–O (benzoyl) distance [mean 1.974 Å]. The dihedral angles between the mean planes of the central phenolato rings (C1A–C6A; C1B–C6B; C1C–C6C) and the peripheral phenyl rings (C9A–C14A & C16A–C21A; C9B–C14B & C16B–C21B; C9C–C14C & C16C–C21C) are 46.62 (10)° & 87.06 (9)°; 60.44 (8)° & 23.13 (8)° and 46.49 (6)° & 65.29 (6)°, respectively, indicating that there is no conjugation between the phenolato and phenyl rings in the mdbp ligands. Further, there are significant differences in the O–C–C–C torsion angles, O1A/C1A/C2A/C8A (–9.9 (4)°), O1B/C1B/C2B/C8B (–2.1 (4)°) and O1C/C1C/C2C/C8C (3.8 (4)°) than that observed in the ligand, O1/C1/C2/C8 (0.0 (3)°) (Gupta *et al.*, 2002) which suggest that distortions are driven by steric interactions. The crystal packing is stabilized by weak C–H···O intermolecular interactions (Fig.2, Table 1). Molecules are further linked by two $\pi$–$\pi$ [*Cg*2–*Cg*10 = 3.9479 (14) Å, *Cg*7—*Cg*7i = 3.8612 (14) Å, symmetry code (i): 1 - *x*, -*y*, -*z*, where *Cg*2, *Cg*7 and *Cg*10 are the centroids of the phenolate (Co/O1B/C1B/C2B/C8B/O2B), and phenyl (C9A–C14A, C16A–C21A) rings, respectively and four C–H···$\pi$ (C10B–H10B–*Cg*12 = 3.634 (3) Å, C11B–H11B–*Cg*7i = 3.479 (3) Å, C18C–H18C–*Cg*9i = 3.720 (4) Å, C20C–H20C–*Cg*11ii = 3.332 (3) Å, symmetry code (i): 1 + *x*, *y*, *z*; ii: 2 - *x*, -1/2 + *y*, +1/2 - *z* where *Cg*9, *Cg*11 and cg12 are the centroids of phenyl (C9C–C14C, C16B–C21B, C16C–C21C rings)) interactions to form a three-dimensional network.

### 2. Experimental

An ethanolic solution of $Co(ClO_4)_2.6H_2O$ (0.366 g, 1.00 mmol) was added dropwise to the stirred hot solution of 2,6-dibenzoyl-4-methylphenol (0.948 g, 3.00 mmol) in ethanol under argon. The resulting wine-red solution was heated to

reflux at 70–80 °C. The clear solution thus obtained was filtered and allowed to cool at ambient temperature. Slow evaporation of the solvent resulted in dark-brown prism-shaped crystals within a few days (yield: 0.80 g, 80%; m.p. 260–262 °C). Analysis calculated for $C_{63}H_{45}O_9Co$ (%): C 75.29, H 4.51; found: C 75.40, H 4.60.

### 3. Refinement

H atoms were positioned geometrically and refined using the riding model, with C–H distance of 0.95–0.98 Å, with $U_{iso}$ (H) = 1.20 $U_{eq}$ (C) or 1.50 $U_{eq}$ (C) for methyl H atoms.

### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

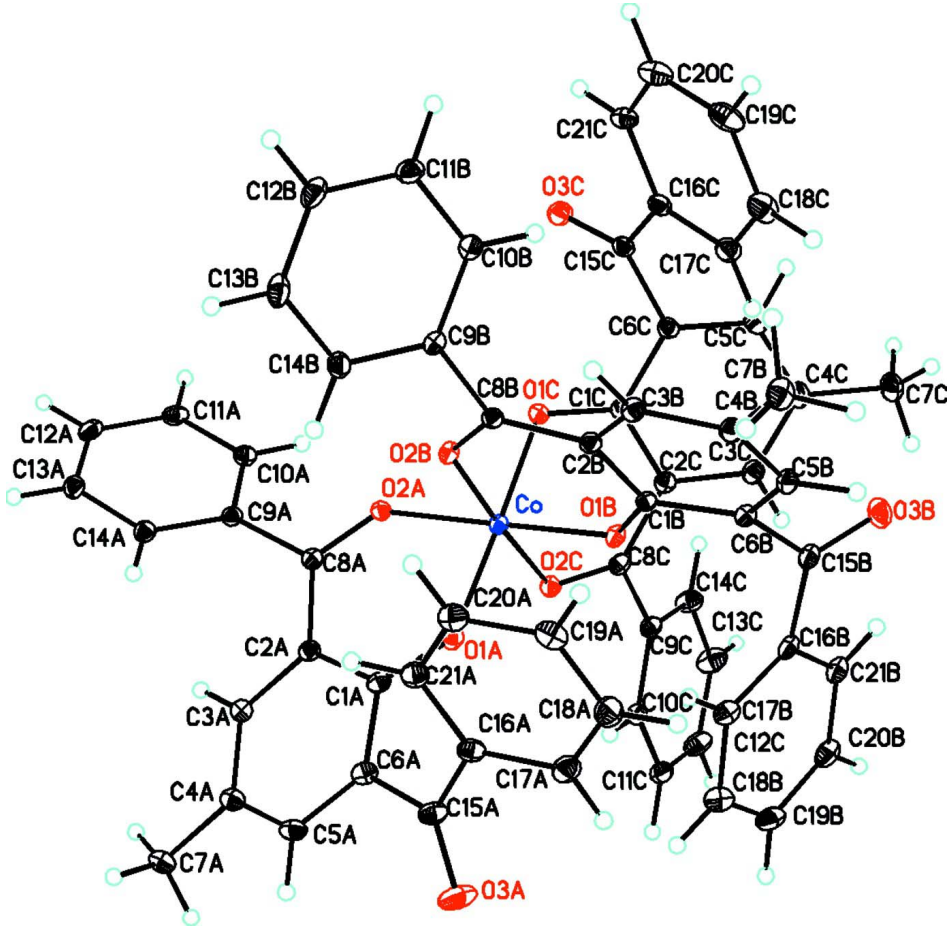


**Figure 1**

Molecular structure of the title compound showing atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

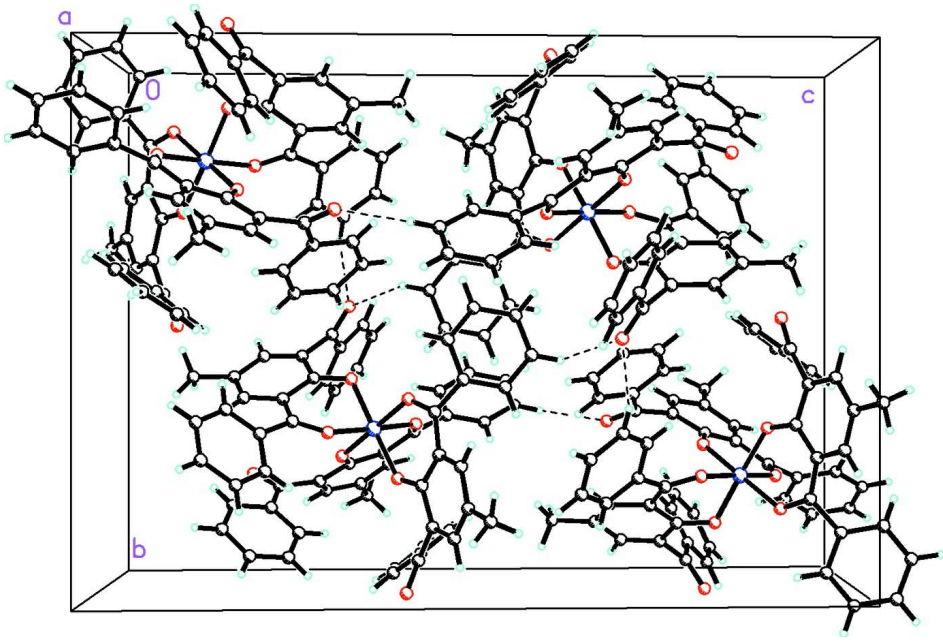


**Figure 2**

Packing diagram of $[Co(C_{21}H_{15}O_3)_3]$ viewed along *a* axis. Dashes lines indicate a weak C–H···O intermolecular interactions.

**Tris(2,6-dibenzoyl-4-methylphenolato-$\kappa^2O^1,O^2$)cobalt(III)**

*Crystal data*

$[Co(C_{21}H_{15}O_3)_3]$
$M_r$ = 1004.92
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 11.2858 (3) Å
$b$ = 17.5442 (4) Å
$c$ = 24.7745 (5) Å
$\beta$ = 92.8922 (19)°
$V$ = 4899.12 (19) Å$^3$
$Z$ = 4
$F(000)$ = 2088
$D_x$ = 1.362 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54184 Å
Cell parameters from 9359 reflections
$\theta$ = 3.1–77.4°
$\mu$ = 3.25 mm$^{-1}$
$T$ = 123 K
Prism, dark brown
0.46 × 0.18 × 0.15 mm

*Data collection*

Agilent Xcalibur (Ruby, Gemini) diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: analytical [*CrysAlis PRO* (Agilent, 2012), based on expressions derived by Clark & Reid (1995)]
$T_{min}$ = 0.477, $T_{max}$ = 0.705
21885 measured reflections
10145 independent reflections
9001 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.045
$\theta_{max}$ = 77.6°, $\theta_{min}$ = 3.6°
$h$ = −13→14
$k$ = −21→15
$l$ = −31→24

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.154$
$S = 1.06$
10145 reflections
661 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0765P)^2 + 3.7684P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.51$ e Å$^{-3}$
$\Delta\rho_{min} = -0.62$ e Å$^{-3}$

*Special details*

**Experimental**. CrysAlisPro (Agilent Technologies, 2012) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897)

**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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Co | 0.38732 (3) | 0.70424 (2) | 0.356917 (14) | 0.01928 (11) |
| O1A | 0.45006 (16) | 0.79710 (9) | 0.39056 (7) | 0.0241 (4) |
| O2A | 0.49775 (14) | 0.64526 (9) | 0.40544 (6) | 0.0219 (3) |
| O3A | 0.5460 (2) | 1.00708 (13) | 0.40380 (12) | 0.0520 (6) |
| C1A | 0.5392 (2) | 0.80635 (14) | 0.42384 (10) | 0.0226 (5) |
| C2A | 0.6100 (2) | 0.74622 (14) | 0.44765 (9) | 0.0227 (5) |
| C3A | 0.7176 (2) | 0.76390 (15) | 0.47654 (10) | 0.0246 (5) |
| H3AA | 0.7663 | 0.7233 | 0.4901 | 0.030* |
| C4A | 0.7548 (2) | 0.83833 (15) | 0.48580 (10) | 0.0265 (5) |
| C5A | 0.6786 (2) | 0.89697 (15) | 0.46756 (10) | 0.0282 (5) |
| H5AA | 0.7003 | 0.9483 | 0.4753 | 0.034* |
| C6A | 0.5727 (2) | 0.88278 (14) | 0.43856 (10) | 0.0261 (5) |
| C7A | 0.8731 (2) | 0.85516 (16) | 0.51452 (11) | 0.0316 (5) |
| H7AA | 0.9184 | 0.8078 | 0.5192 | 0.047* |
| H7AB | 0.8603 | 0.8775 | 0.5500 | 0.047* |
| H7AC | 0.9175 | 0.8912 | 0.4930 | 0.047* |
| C8A | 0.5713 (2) | 0.66727 (14) | 0.44132 (9) | 0.0218 (4) |
| C9A | 0.6168 (2) | 0.60673 (14) | 0.47901 (9) | 0.0223 (5) |
| C10A | 0.6254 (2) | 0.53247 (14) | 0.45905 (10) | 0.0253 (5) |
| H10A | 0.6044 | 0.5222 | 0.4222 | 0.030* |
| C11A | 0.6646 (2) | 0.47389 (14) | 0.49288 (11) | 0.0291 (5) |
| H11A | 0.6729 | 0.4239 | 0.4788 | 0.035* |
| C12A | 0.6918 (2) | 0.48798 (16) | 0.54746 (11) | 0.0306 (5) |

| | | | | |
|---|---|---|---|---|
| H12A | 0.7191 | 0.4477 | 0.5706 | 0.037* |
| C13A | 0.6790 (2) | 0.56087 (16) | 0.56794 (10) | 0.0277 (5) |
| H13A | 0.6955 | 0.5702 | 0.6053 | 0.033* |
| C14A | 0.6423 (2) | 0.62031 (15) | 0.53404 (10) | 0.0244 (5) |
| H14A | 0.6344 | 0.6703 | 0.5482 | 0.029* |
| C15A | 0.4986 (2) | 0.94882 (15) | 0.41900 (12) | 0.0317 (5) |
| C16A | 0.3663 (2) | 0.94498 (14) | 0.42014 (11) | 0.0282 (5) |
| C17A | 0.2985 (3) | 0.98635 (16) | 0.38188 (12) | 0.0340 (6) |
| H17A | 0.3370 | 1.0149 | 0.3553 | 0.041* |
| C18A | 0.1754 (3) | 0.98642 (17) | 0.38207 (12) | 0.0373 (6) |
| H18A | 0.1298 | 1.0135 | 0.3551 | 0.045* |
| C19A | 0.1197 (2) | 0.94677 (17) | 0.42181 (12) | 0.0348 (6) |
| H19A | 0.0357 | 0.9474 | 0.4226 | 0.042* |
| C20A | 0.1863 (3) | 0.90615 (16) | 0.46045 (11) | 0.0329 (6) |
| H20A | 0.1476 | 0.8794 | 0.4878 | 0.040* |
| C21A | 0.3092 (2) | 0.90421 (15) | 0.45952 (11) | 0.0303 (5) |
| H21A | 0.3541 | 0.8752 | 0.4856 | 0.036* |
| O1B | 0.27825 (14) | 0.76059 (10) | 0.31121 (6) | 0.0218 (3) |
| O2B | 0.26886 (15) | 0.69853 (9) | 0.41242 (7) | 0.0222 (3) |
| O3B | 0.09769 (18) | 0.80141 (14) | 0.18133 (8) | 0.0405 (5) |
| C1B | 0.1695 (2) | 0.77906 (13) | 0.31834 (9) | 0.0197 (4) |
| C2B | 0.1057 (2) | 0.76091 (13) | 0.36543 (9) | 0.0212 (4) |
| C3B | −0.0114 (2) | 0.78836 (14) | 0.36943 (10) | 0.0235 (5) |
| H3BA | −0.0516 | 0.7780 | 0.4014 | 0.028* |
| C4B | −0.0695 (2) | 0.82958 (14) | 0.32878 (10) | 0.0257 (5) |
| C5B | −0.0102 (2) | 0.84059 (14) | 0.28079 (10) | 0.0256 (5) |
| H5BA | −0.0511 | 0.8652 | 0.2512 | 0.031* |
| C6B | 0.1049 (2) | 0.81700 (14) | 0.27515 (9) | 0.0230 (5) |
| C7B | −0.1936 (2) | 0.85986 (18) | 0.33490 (12) | 0.0339 (6) |
| H7BA | −0.2464 | 0.8177 | 0.3435 | 0.051* |
| H7BB | −0.2224 | 0.8839 | 0.3010 | 0.051* |
| H7BC | −0.1925 | 0.8975 | 0.3641 | 0.051* |
| C8B | 0.1611 (2) | 0.71668 (13) | 0.40888 (9) | 0.0202 (4) |
| C9B | 0.0913 (2) | 0.68677 (14) | 0.45423 (9) | 0.0221 (4) |
| C10B | −0.0060 (2) | 0.63968 (15) | 0.44322 (10) | 0.0272 (5) |
| H10B | −0.0347 | 0.6318 | 0.4069 | 0.033* |
| C11B | −0.0611 (2) | 0.60415 (17) | 0.48537 (12) | 0.0330 (6) |
| H11B | −0.1253 | 0.5701 | 0.4779 | 0.040* |
| C12B | −0.0223 (2) | 0.61863 (19) | 0.53844 (11) | 0.0379 (7) |
| H12B | −0.0614 | 0.5955 | 0.5673 | 0.045* |
| C13B | 0.0732 (2) | 0.6666 (2) | 0.54952 (11) | 0.0366 (6) |
| H13B | 0.0984 | 0.6771 | 0.5859 | 0.044* |
| C14B | 0.1321 (2) | 0.69935 (15) | 0.50742 (10) | 0.0279 (5) |
| H14B | 0.2000 | 0.7303 | 0.5149 | 0.034* |
| C15B | 0.1576 (2) | 0.82364 (15) | 0.22050 (10) | 0.0264 (5) |
| C16B | 0.2749 (2) | 0.86002 (15) | 0.21381 (10) | 0.0267 (5) |
| C17B | 0.3289 (2) | 0.90612 (16) | 0.25359 (11) | 0.0321 (6) |
| H17B | 0.2956 | 0.9099 | 0.2879 | 0.039* |
| C18B | 0.4309 (3) | 0.94661 (17) | 0.24345 (13) | 0.0387 (6) |

| | | | | |
|---|---|---|---|---|
| H18B | 0.4663 | 0.9787 | 0.2706 | 0.046* |
| C19B | 0.4817 (3) | 0.94033 (17) | 0.19372 (13) | 0.0372 (6) |
| H19B | 0.5509 | 0.9687 | 0.1866 | 0.045* |
| C20B | 0.4305 (2) | 0.89232 (17) | 0.15445 (12) | 0.0345 (6) |
| H20B | 0.4663 | 0.8867 | 0.1208 | 0.041* |
| C21B | 0.3280 (2) | 0.85279 (16) | 0.16411 (11) | 0.0296 (5) |
| H21B | 0.2932 | 0.8205 | 0.1369 | 0.035* |
| O1C | 0.32753 (15) | 0.60991 (10) | 0.32491 (6) | 0.0229 (3) |
| O2C | 0.49974 (15) | 0.70749 (10) | 0.29840 (7) | 0.0230 (3) |
| O3C | 0.16902 (17) | 0.46986 (11) | 0.31788 (8) | 0.0331 (4) |
| C1C | 0.3010 (2) | 0.60812 (13) | 0.27299 (9) | 0.0214 (4) |
| C2C | 0.3681 (2) | 0.64691 (14) | 0.23363 (10) | 0.0241 (5) |
| C3C | 0.3266 (2) | 0.64560 (15) | 0.17862 (10) | 0.0278 (5) |
| H3CA | 0.3704 | 0.6725 | 0.1529 | 0.033* |
| C4C | 0.2259 (3) | 0.60711 (17) | 0.16093 (10) | 0.0317 (6) |
| C5C | 0.1635 (2) | 0.56738 (16) | 0.19942 (10) | 0.0293 (5) |
| H5CA | 0.0942 | 0.5399 | 0.1879 | 0.035* |
| C6C | 0.1993 (2) | 0.56678 (14) | 0.25364 (10) | 0.0238 (5) |
| C7C | 0.1833 (3) | 0.6079 (2) | 0.10236 (11) | 0.0433 (7) |
| H7CA | 0.2346 | 0.6411 | 0.0820 | 0.065* |
| H7CB | 0.1016 | 0.6270 | 0.0992 | 0.065* |
| H7CC | 0.1858 | 0.5560 | 0.0878 | 0.065* |
| C8C | 0.4756 (2) | 0.68717 (14) | 0.25044 (10) | 0.0232 (5) |
| C9C | 0.5663 (2) | 0.70757 (14) | 0.21124 (10) | 0.0254 (5) |
| C10C | 0.6301 (2) | 0.77469 (15) | 0.22062 (10) | 0.0277 (5) |
| H10C | 0.6129 | 0.8063 | 0.2504 | 0.033* |
| C11C | 0.7187 (3) | 0.79563 (16) | 0.18670 (12) | 0.0338 (6) |
| H11C | 0.7617 | 0.8416 | 0.1931 | 0.041* |
| C12C | 0.7444 (3) | 0.74934 (19) | 0.14349 (13) | 0.0413 (7) |
| H12C | 0.8059 | 0.7632 | 0.1206 | 0.050* |
| C13C | 0.6805 (3) | 0.68285 (19) | 0.13359 (13) | 0.0422 (7) |
| H13C | 0.6976 | 0.6516 | 0.1036 | 0.051* |
| C14C | 0.5913 (3) | 0.66184 (16) | 0.16748 (12) | 0.0343 (6) |
| H14C | 0.5476 | 0.6163 | 0.1607 | 0.041* |
| C15C | 0.1273 (2) | 0.52477 (14) | 0.29308 (10) | 0.0244 (5) |
| C16C | 0.0036 (2) | 0.55076 (14) | 0.30089 (10) | 0.0250 (5) |
| C17C | −0.0408 (2) | 0.61907 (15) | 0.27878 (11) | 0.0305 (5) |
| H17C | 0.0077 | 0.6498 | 0.2573 | 0.037* |
| C18C | −0.1556 (3) | 0.64190 (18) | 0.28816 (14) | 0.0397 (7) |
| H18C | −0.1855 | 0.6882 | 0.2730 | 0.048* |
| C19C | −0.2271 (3) | 0.59739 (19) | 0.31970 (14) | 0.0417 (7) |
| H19C | −0.3056 | 0.6133 | 0.3262 | 0.050* |
| C20C | −0.1829 (3) | 0.52935 (18) | 0.34171 (13) | 0.0390 (7) |
| H20C | −0.2314 | 0.4988 | 0.3633 | 0.047* |
| C21C | −0.0688 (2) | 0.50623 (15) | 0.33220 (11) | 0.0301 (5) |
| H21C | −0.0394 | 0.4596 | 0.3471 | 0.036* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co | 0.0200 (2) | 0.0188 (2) | 0.01894 (19) | 0.00065 (14) | 0.00017 (13) | 0.00137 (14) |
| O1A | 0.0307 (9) | 0.0180 (8) | 0.0235 (8) | 0.0033 (6) | −0.0002 (7) | 0.0001 (6) |
| O2A | 0.0243 (8) | 0.0183 (8) | 0.0228 (8) | −0.0010 (6) | −0.0029 (6) | 0.0006 (6) |
| O3A | 0.0395 (12) | 0.0282 (11) | 0.0885 (18) | −0.0021 (9) | 0.0051 (11) | 0.0192 (11) |
| C1A | 0.0228 (11) | 0.0203 (11) | 0.0254 (11) | 0.0004 (9) | 0.0065 (9) | 0.0006 (9) |
| C2A | 0.0256 (11) | 0.0199 (11) | 0.0227 (11) | 0.0001 (9) | 0.0032 (8) | −0.0004 (9) |
| C3A | 0.0237 (11) | 0.0248 (12) | 0.0255 (11) | 0.0019 (9) | 0.0028 (9) | −0.0005 (9) |
| C4A | 0.0236 (11) | 0.0279 (13) | 0.0283 (12) | −0.0022 (10) | 0.0057 (9) | −0.0039 (10) |
| C5A | 0.0308 (13) | 0.0221 (12) | 0.0324 (13) | −0.0045 (10) | 0.0080 (10) | −0.0049 (10) |
| C6A | 0.0267 (12) | 0.0216 (12) | 0.0306 (12) | 0.0018 (9) | 0.0073 (9) | −0.0006 (9) |
| C7A | 0.0289 (13) | 0.0310 (13) | 0.0351 (13) | −0.0049 (10) | 0.0021 (10) | −0.0078 (11) |
| C8A | 0.0196 (10) | 0.0236 (12) | 0.0225 (11) | 0.0009 (9) | 0.0041 (8) | 0.0005 (9) |
| C9A | 0.0197 (10) | 0.0220 (11) | 0.0254 (11) | −0.0006 (9) | 0.0017 (8) | 0.0022 (9) |
| C10A | 0.0229 (11) | 0.0230 (12) | 0.0302 (12) | −0.0002 (9) | 0.0022 (9) | −0.0001 (9) |
| C11A | 0.0271 (12) | 0.0179 (11) | 0.0424 (14) | 0.0010 (9) | 0.0033 (10) | 0.0030 (10) |
| C12A | 0.0261 (12) | 0.0279 (13) | 0.0378 (14) | −0.0006 (10) | 0.0014 (10) | 0.0142 (11) |
| C13A | 0.0227 (11) | 0.0354 (14) | 0.0250 (11) | −0.0021 (10) | 0.0001 (9) | 0.0057 (10) |
| C14A | 0.0234 (11) | 0.0251 (12) | 0.0248 (11) | 0.0000 (9) | 0.0022 (9) | 0.0012 (9) |
| C15A | 0.0345 (14) | 0.0186 (12) | 0.0422 (14) | 0.0000 (10) | 0.0052 (11) | 0.0010 (10) |
| C16A | 0.0329 (13) | 0.0174 (11) | 0.0345 (13) | 0.0002 (10) | 0.0025 (10) | −0.0046 (10) |
| C17A | 0.0398 (15) | 0.0253 (13) | 0.0369 (14) | 0.0027 (11) | 0.0029 (11) | 0.0014 (11) |
| C18A | 0.0386 (15) | 0.0316 (14) | 0.0412 (15) | 0.0050 (12) | −0.0039 (12) | 0.0014 (12) |
| C19A | 0.0276 (13) | 0.0315 (14) | 0.0453 (15) | 0.0009 (11) | 0.0014 (11) | −0.0084 (12) |
| C20A | 0.0353 (14) | 0.0304 (14) | 0.0336 (13) | −0.0008 (11) | 0.0064 (11) | −0.0043 (11) |
| C21A | 0.0338 (13) | 0.0237 (12) | 0.0336 (13) | 0.0011 (10) | 0.0027 (10) | −0.0031 (10) |
| O1B | 0.0217 (8) | 0.0233 (8) | 0.0205 (7) | 0.0031 (6) | 0.0024 (6) | 0.0048 (6) |
| O2B | 0.0236 (8) | 0.0235 (8) | 0.0194 (8) | 0.0016 (6) | 0.0011 (6) | 0.0034 (6) |
| O3B | 0.0351 (11) | 0.0653 (15) | 0.0208 (9) | −0.0087 (10) | −0.0006 (7) | 0.0042 (9) |
| C1B | 0.0215 (11) | 0.0163 (10) | 0.0211 (10) | 0.0000 (8) | −0.0002 (8) | 0.0008 (8) |
| C2B | 0.0240 (11) | 0.0191 (11) | 0.0206 (10) | −0.0010 (9) | 0.0013 (8) | −0.0007 (8) |
| C3B | 0.0256 (12) | 0.0245 (12) | 0.0208 (11) | 0.0003 (9) | 0.0039 (9) | −0.0008 (9) |
| C4B | 0.0241 (12) | 0.0230 (12) | 0.0299 (12) | 0.0014 (9) | 0.0004 (9) | 0.0020 (9) |
| C5B | 0.0243 (11) | 0.0246 (12) | 0.0274 (12) | 0.0028 (9) | −0.0030 (9) | 0.0054 (9) |
| C6B | 0.0257 (12) | 0.0207 (11) | 0.0226 (11) | −0.0010 (9) | 0.0002 (9) | 0.0027 (9) |
| C7B | 0.0259 (12) | 0.0411 (15) | 0.0349 (14) | 0.0081 (11) | 0.0034 (10) | 0.0052 (12) |
| C8B | 0.0237 (11) | 0.0179 (10) | 0.0192 (10) | −0.0016 (8) | 0.0024 (8) | −0.0017 (8) |
| C9B | 0.0241 (11) | 0.0212 (11) | 0.0212 (11) | 0.0020 (9) | 0.0029 (8) | 0.0030 (9) |
| C10B | 0.0276 (12) | 0.0283 (12) | 0.0256 (12) | −0.0003 (10) | 0.0005 (9) | 0.0026 (10) |
| C11B | 0.0239 (12) | 0.0346 (14) | 0.0407 (14) | −0.0033 (10) | 0.0034 (10) | 0.0106 (12) |
| C12B | 0.0274 (13) | 0.0556 (19) | 0.0313 (13) | 0.0029 (12) | 0.0067 (10) | 0.0189 (13) |
| C13B | 0.0306 (13) | 0.0591 (19) | 0.0201 (11) | 0.0046 (13) | 0.0016 (10) | 0.0069 (12) |
| C14B | 0.0268 (12) | 0.0340 (14) | 0.0230 (12) | −0.0009 (10) | 0.0005 (9) | 0.0009 (10) |
| C15B | 0.0282 (12) | 0.0268 (12) | 0.0241 (12) | 0.0036 (10) | −0.0001 (9) | 0.0071 (9) |
| C16B | 0.0299 (12) | 0.0249 (12) | 0.0252 (11) | 0.0036 (10) | 0.0018 (9) | 0.0101 (9) |
| C17B | 0.0340 (14) | 0.0298 (13) | 0.0330 (13) | −0.0019 (11) | 0.0060 (10) | 0.0049 (11) |
| C18B | 0.0396 (15) | 0.0323 (15) | 0.0445 (16) | −0.0046 (12) | 0.0044 (12) | 0.0008 (12) |
| C19B | 0.0308 (14) | 0.0308 (14) | 0.0507 (17) | −0.0026 (11) | 0.0099 (12) | 0.0103 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C20B | 0.0326 (13) | 0.0368 (15) | 0.0350 (14) | 0.0075 (11) | 0.0103 (11) | 0.0121 (11) |
| C21B | 0.0294 (12) | 0.0317 (13) | 0.0277 (12) | 0.0062 (10) | 0.0029 (10) | 0.0087 (10) |
| O1C | 0.0256 (8) | 0.0210 (8) | 0.0219 (8) | −0.0029 (6) | −0.0016 (6) | −0.0004 (6) |
| O2C | 0.0221 (8) | 0.0244 (9) | 0.0226 (8) | 0.0004 (6) | 0.0018 (6) | 0.0005 (6) |
| O3C | 0.0320 (10) | 0.0247 (9) | 0.0420 (10) | 0.0010 (8) | −0.0037 (8) | 0.0058 (8) |
| C1C | 0.0210 (11) | 0.0205 (11) | 0.0226 (11) | 0.0006 (9) | −0.0004 (8) | −0.0011 (9) |
| C2C | 0.0262 (11) | 0.0213 (11) | 0.0249 (11) | 0.0021 (9) | 0.0018 (9) | −0.0013 (9) |
| C3C | 0.0324 (13) | 0.0288 (13) | 0.0226 (11) | 0.0015 (10) | 0.0036 (9) | −0.0001 (9) |
| C4C | 0.0374 (14) | 0.0350 (14) | 0.0223 (11) | 0.0018 (11) | −0.0033 (10) | −0.0015 (10) |
| C5C | 0.0285 (12) | 0.0302 (13) | 0.0289 (12) | −0.0031 (10) | −0.0032 (9) | −0.0053 (10) |
| C6C | 0.0226 (11) | 0.0216 (11) | 0.0269 (11) | 0.0002 (9) | 0.0002 (9) | −0.0013 (9) |
| C7C | 0.0485 (17) | 0.0557 (19) | 0.0249 (13) | −0.0068 (15) | −0.0050 (12) | 0.0002 (13) |
| C8C | 0.0251 (12) | 0.0187 (11) | 0.0259 (11) | 0.0047 (9) | 0.0035 (9) | 0.0015 (9) |
| C9C | 0.0252 (12) | 0.0239 (12) | 0.0273 (12) | 0.0025 (9) | 0.0040 (9) | 0.0028 (9) |
| C10C | 0.0298 (12) | 0.0249 (12) | 0.0282 (12) | −0.0001 (10) | −0.0019 (9) | 0.0037 (10) |
| C11C | 0.0311 (14) | 0.0313 (14) | 0.0389 (15) | −0.0044 (11) | −0.0007 (11) | 0.0088 (11) |
| C12C | 0.0408 (16) | 0.0409 (16) | 0.0437 (16) | −0.0028 (13) | 0.0172 (12) | 0.0117 (13) |
| C13C | 0.0497 (18) | 0.0371 (16) | 0.0420 (16) | 0.0002 (14) | 0.0234 (14) | −0.0006 (13) |
| C14C | 0.0384 (15) | 0.0276 (13) | 0.0380 (14) | −0.0024 (11) | 0.0135 (11) | −0.0014 (11) |
| C15C | 0.0253 (11) | 0.0204 (11) | 0.0271 (11) | −0.0028 (9) | −0.0032 (9) | −0.0031 (9) |
| C16C | 0.0240 (11) | 0.0220 (11) | 0.0287 (12) | −0.0027 (9) | −0.0025 (9) | −0.0031 (9) |
| C17C | 0.0284 (12) | 0.0244 (12) | 0.0380 (14) | 0.0003 (10) | −0.0032 (10) | −0.0006 (10) |
| C18C | 0.0306 (14) | 0.0328 (15) | 0.0550 (18) | 0.0074 (11) | −0.0058 (12) | −0.0044 (13) |
| C19C | 0.0243 (13) | 0.0443 (17) | 0.0567 (18) | −0.0012 (12) | 0.0039 (12) | −0.0182 (14) |
| C20C | 0.0339 (14) | 0.0375 (16) | 0.0462 (16) | −0.0108 (12) | 0.0096 (12) | −0.0122 (13) |
| C21C | 0.0304 (13) | 0.0256 (12) | 0.0343 (13) | −0.0076 (10) | 0.0032 (10) | −0.0033 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Co—O1B | 1.9063 (16) | C9B—C10B | 1.390 (4) |
| Co—O1C | 1.9414 (17) | C9B—C14B | 1.391 (3) |
| Co—O1A | 1.9470 (17) | C10B—C11B | 1.390 (4) |
| Co—O2B | 1.9682 (17) | C10B—H10B | 0.9500 |
| Co—O2C | 1.9749 (17) | C11B—C12B | 1.388 (4) |
| Co—O2A | 1.9793 (16) | C11B—H11B | 0.9500 |
| O1A—C1A | 1.279 (3) | C12B—C13B | 1.383 (4) |
| O2A—C8A | 1.247 (3) | C12B—H12B | 0.9500 |
| O3A—C15A | 1.222 (3) | C13B—C14B | 1.389 (4) |
| C1A—C2A | 1.432 (3) | C13B—H13B | 0.9500 |
| C1A—C6A | 1.435 (3) | C14B—H14B | 0.9500 |
| C2A—C3A | 1.413 (3) | C15B—C16B | 1.487 (4) |
| C2A—C8A | 1.459 (3) | C16B—C17B | 1.391 (4) |
| C3A—C4A | 1.387 (4) | C16B—C21B | 1.402 (4) |
| C3A—H3AA | 0.9500 | C17B—C18B | 1.387 (4) |
| C4A—C5A | 1.401 (4) | C17B—H17B | 0.9500 |
| C4A—C7A | 1.510 (3) | C18B—C19B | 1.389 (4) |
| C5A—C6A | 1.386 (4) | C18B—H18B | 0.9500 |
| C5A—H5AA | 0.9500 | C19B—C20B | 1.390 (4) |
| C6A—C15A | 1.495 (4) | C19B—H19B | 0.9500 |
| C7A—H7AA | 0.9800 | C20B—C21B | 1.380 (4) |

| | | | |
|---|---|---|---|
| C7A—H7AB | 0.9800 | C20B—H20B | 0.9500 |
| C7A—H7AC | 0.9800 | C21B—H21B | 0.9500 |
| C8A—C9A | 1.488 (3) | O1C—C1C | 1.306 (3) |
| C9A—C10A | 1.399 (3) | O2C—C8C | 1.257 (3) |
| C9A—C14A | 1.399 (3) | O3C—C15C | 1.224 (3) |
| C10A—C11A | 1.384 (4) | C1C—C6C | 1.421 (3) |
| C10A—H10A | 0.9500 | C1C—C2C | 1.436 (3) |
| C11A—C12A | 1.394 (4) | C2C—C3C | 1.418 (3) |
| C11A—H11A | 0.9500 | C2C—C8C | 1.447 (3) |
| C12A—C13A | 1.386 (4) | C3C—C4C | 1.375 (4) |
| C12A—H12A | 0.9500 | C3C—H3CA | 0.9500 |
| C13A—C14A | 1.389 (4) | C4C—C5C | 1.400 (4) |
| C13A—H13A | 0.9500 | C4C—C7C | 1.506 (4) |
| C14A—H14A | 0.9500 | C5C—C6C | 1.383 (3) |
| C15A—C16A | 1.497 (4) | C5C—H5CA | 0.9500 |
| C16A—C17A | 1.392 (4) | C6C—C15C | 1.496 (3) |
| C16A—C21A | 1.394 (4) | C7C—H7CA | 0.9800 |
| C17A—C18A | 1.390 (4) | C7C—H7CB | 0.9800 |
| C17A—H17A | 0.9500 | C7C—H7CC | 0.9800 |
| C18A—C19A | 1.382 (4) | C8C—C9C | 1.490 (3) |
| C18A—H18A | 0.9500 | C9C—C14C | 1.389 (4) |
| C19A—C20A | 1.384 (4) | C9C—C10C | 1.394 (4) |
| C19A—H19A | 0.9500 | C10C—C11C | 1.388 (4) |
| C20A—C21A | 1.388 (4) | C10C—H10C | 0.9500 |
| C20A—H20A | 0.9500 | C11C—C12C | 1.386 (5) |
| C21A—H21A | 0.9500 | C11C—H11C | 0.9500 |
| O1B—C1B | 1.290 (3) | C12C—C13C | 1.387 (5) |
| O2B—C8B | 1.256 (3) | C12C—H12C | 0.9500 |
| O3B—C15B | 1.219 (3) | C13C—C14C | 1.392 (4) |
| C1B—C6B | 1.429 (3) | C13C—H13C | 0.9500 |
| C1B—C2B | 1.437 (3) | C14C—H14C | 0.9500 |
| C2B—C3B | 1.415 (3) | C15C—C16C | 1.491 (3) |
| C2B—C8B | 1.443 (3) | C16C—C21C | 1.394 (4) |
| C3B—C4B | 1.379 (3) | C16C—C17C | 1.400 (4) |
| C3B—H3BA | 0.9500 | C17C—C18C | 1.387 (4) |
| C4B—C5B | 1.407 (3) | C17C—H17C | 0.9500 |
| C4B—C7B | 1.513 (3) | C18C—C19C | 1.391 (5) |
| C5B—C6B | 1.377 (3) | C18C—H18C | 0.9500 |
| C5B—H5BA | 0.9500 | C19C—C20C | 1.394 (5) |
| C6B—C15B | 1.511 (3) | C19C—H19C | 0.9500 |
| C7B—H7BA | 0.9800 | C20C—C21C | 1.382 (4) |
| C7B—H7BB | 0.9800 | C20C—H20C | 0.9500 |
| C7B—H7BC | 0.9800 | C21C—H21C | 0.9500 |
| C8B—C9B | 1.499 (3) | | |

| | | | |
|---|---|---|---|
| O1B—Co—O1C | 89.93 (7) | O2B—C8B—C9B | 113.7 (2) |
| O1B—Co—O1A | 91.73 (7) | C2B—C8B—C9B | 121.5 (2) |
| O1C—Co—O1A | 178.32 (7) | C10B—C9B—C14B | 120.0 (2) |
| O1B—Co—O2B | 90.02 (7) | C10B—C9B—C8B | 120.0 (2) |

| | | | |
|---|---|---|---|
| O1C—Co—O2B | 90.44 (7) | C14B—C9B—C8B | 119.5 (2) |
| O1A—Co—O2B | 89.35 (7) | C11B—C10B—C9B | 119.9 (2) |
| O1B—Co—O2C | 88.19 (7) | C11B—C10B—H10B | 120.1 |
| O1C—Co—O2C | 87.01 (7) | C9B—C10B—H10B | 120.1 |
| O1A—Co—O2C | 93.25 (7) | C12B—C11B—C10B | 119.8 (3) |
| O2B—Co—O2C | 176.88 (7) | C12B—C11B—H11B | 120.1 |
| O1B—Co—O2A | 178.76 (7) | C10B—C11B—H11B | 120.1 |
| O1C—Co—O2A | 89.87 (7) | C13B—C12B—C11B | 120.3 (2) |
| O1A—Co—O2A | 88.47 (7) | C13B—C12B—H12B | 119.8 |
| O2B—Co—O2A | 88.75 (7) | C11B—C12B—H12B | 119.8 |
| O2C—Co—O2A | 93.02 (7) | C12B—C13B—C14B | 120.0 (3) |
| C1A—O1A—Co | 129.76 (16) | C12B—C13B—H13B | 120.0 |
| C8A—O2A—Co | 130.35 (16) | C14B—C13B—H13B | 120.0 |
| O1A—C1A—C2A | 125.2 (2) | C13B—C14B—C9B | 119.8 (2) |
| O1A—C1A—C6A | 118.1 (2) | C13B—C14B—H14B | 120.1 |
| C2A—C1A—C6A | 116.7 (2) | C9B—C14B—H14B | 120.1 |
| C3A—C2A—C1A | 119.6 (2) | O3B—C15B—C16B | 120.7 (2) |
| C3A—C2A—C8A | 120.6 (2) | O3B—C15B—C6B | 117.5 (2) |
| C1A—C2A—C8A | 119.8 (2) | C16B—C15B—C6B | 121.8 (2) |
| C4A—C3A—C2A | 122.4 (2) | C17B—C16B—C21B | 118.9 (2) |
| C4A—C3A—H3AA | 118.8 | C17B—C16B—C15B | 122.1 (2) |
| C2A—C3A—H3AA | 118.8 | C21B—C16B—C15B | 118.8 (2) |
| C3A—C4A—C5A | 117.5 (2) | C18B—C17B—C16B | 120.5 (3) |
| C3A—C4A—C7A | 121.0 (2) | C18B—C17B—H17B | 119.8 |
| C5A—C4A—C7A | 121.5 (2) | C16B—C17B—H17B | 119.8 |
| C6A—C5A—C4A | 122.3 (2) | C17B—C18B—C19B | 120.2 (3) |
| C6A—C5A—H5AA | 118.8 | C17B—C18B—H18B | 119.9 |
| C4A—C5A—H5AA | 118.8 | C19B—C18B—H18B | 119.9 |
| C5A—C6A—C1A | 120.5 (2) | C18B—C19B—C20B | 119.6 (3) |
| C5A—C6A—C15A | 118.8 (2) | C18B—C19B—H19B | 120.2 |
| C1A—C6A—C15A | 120.4 (2) | C20B—C19B—H19B | 120.2 |
| C4A—C7A—H7AA | 109.5 | C21B—C20B—C19B | 120.3 (3) |
| C4A—C7A—H7AB | 109.5 | C21B—C20B—H20B | 119.8 |
| H7AA—C7A—H7AB | 109.5 | C19B—C20B—H20B | 119.8 |
| C4A—C7A—H7AC | 109.5 | C20B—C21B—C16B | 120.4 (3) |
| H7AA—C7A—H7AC | 109.5 | C20B—C21B—H21B | 119.8 |
| H7AB—C7A—H7AC | 109.5 | C16B—C21B—H21B | 119.8 |
| O2A—C8A—C2A | 123.8 (2) | C1C—O1C—Co | 118.70 (15) |
| O2A—C8A—C9A | 115.0 (2) | C8C—O2C—Co | 124.66 (16) |
| C2A—C8A—C9A | 121.2 (2) | O1C—C1C—C6C | 119.0 (2) |
| C10A—C9A—C14A | 119.2 (2) | O1C—C1C—C2C | 123.7 (2) |
| C10A—C9A—C8A | 118.1 (2) | C6C—C1C—C2C | 117.2 (2) |
| C14A—C9A—C8A | 122.5 (2) | C3C—C2C—C1C | 119.0 (2) |
| C11A—C10A—C9A | 120.2 (2) | C3C—C2C—C8C | 121.0 (2) |
| C11A—C10A—H10A | 119.9 | C1C—C2C—C8C | 119.9 (2) |
| C9A—C10A—H10A | 119.9 | C4C—C3C—C2C | 122.8 (2) |
| C10A—C11A—C12A | 120.3 (2) | C4C—C3C—H3CA | 118.6 |
| C10A—C11A—H11A | 119.9 | C2C—C3C—H3CA | 118.6 |
| C12A—C11A—H11A | 119.9 | C3C—C4C—C5C | 117.6 (2) |

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| C13A—C12A—C11A | 119.8 (2) | C3C—C4C—C7C | 121.5 (3) |
| C13A—C12A—H12A | 120.1 | C5C—C4C—C7C | 120.9 (3) |
| C11A—C12A—H12A | 120.1 | C6C—C5C—C4C | 122.2 (2) |
| C12A—C13A—C14A | 120.3 (2) | C6C—C5C—H5CA | 118.9 |
| C12A—C13A—H13A | 119.8 | C4C—C5C—H5CA | 118.9 |
| C14A—C13A—H13A | 119.8 | C5C—C6C—C1C | 121.0 (2) |
| C13A—C14A—C9A | 120.1 (2) | C5C—C6C—C15C | 119.8 (2) |
| C13A—C14A—H14A | 119.9 | C1C—C6C—C15C | 119.2 (2) |
| C9A—C14A—H14A | 119.9 | C4C—C7C—H7CA | 109.5 |
| O3A—C15A—C6A | 120.2 (3) | C4C—C7C—H7CB | 109.5 |
| O3A—C15A—C16A | 119.7 (3) | H7CA—C7C—H7CB | 109.5 |
| C6A—C15A—C16A | 120.1 (2) | C4C—C7C—H7CC | 109.5 |
| C17A—C16A—C21A | 119.1 (3) | H7CA—C7C—H7CC | 109.5 |
| C17A—C16A—C15A | 118.6 (2) | H7CB—C7C—H7CC | 109.5 |
| C21A—C16A—C15A | 122.3 (2) | O2C—C8C—C2C | 123.3 (2) |
| C18A—C17A—C16A | 120.9 (3) | O2C—C8C—C9C | 115.1 (2) |
| C18A—C17A—H17A | 119.6 | C2C—C8C—C9C | 121.6 (2) |
| C16A—C17A—H17A | 119.6 | C14C—C9C—C10C | 119.6 (2) |
| C19A—C18A—C17A | 119.5 (3) | C14C—C9C—C8C | 122.9 (2) |
| C19A—C18A—H18A | 120.3 | C10C—C9C—C8C | 117.4 (2) |
| C17A—C18A—H18A | 120.3 | C11C—C10C—C9C | 120.3 (3) |
| C18A—C19A—C20A | 120.1 (3) | C11C—C10C—H10C | 119.8 |
| C18A—C19A—H19A | 120.0 | C9C—C10C—H10C | 119.8 |
| C20A—C19A—H19A | 120.0 | C12C—C11C—C10C | 119.8 (3) |
| C19A—C20A—C21A | 120.6 (3) | C12C—C11C—H11C | 120.1 |
| C19A—C20A—H20A | 119.7 | C10C—C11C—H11C | 120.1 |
| C21A—C20A—H20A | 119.7 | C11C—C12C—C13C | 120.2 (3) |
| C20A—C21A—C16A | 119.8 (3) | C11C—C12C—H12C | 119.9 |
| C20A—C21A—H21A | 120.1 | C13C—C12C—H12C | 119.9 |
| C16A—C21A—H21A | 120.1 | C12C—C13C—C14C | 120.1 (3) |
| C1B—O1B—Co | 129.72 (14) | C12C—C13C—H13C | 120.0 |
| C8B—O2B—Co | 128.88 (15) | C14C—C13C—H13C | 120.0 |
| O1B—C1B—C6B | 117.9 (2) | C9C—C14C—C13C | 120.0 (3) |
| O1B—C1B—C2B | 125.1 (2) | C9C—C14C—H14C | 120.0 |
| C6B—C1B—C2B | 117.0 (2) | C13C—C14C—H14C | 120.0 |
| C3B—C2B—C1B | 119.3 (2) | O3C—C15C—C16C | 121.0 (2) |
| C3B—C2B—C8B | 120.1 (2) | O3C—C15C—C6C | 120.5 (2) |
| C1B—C2B—C8B | 120.6 (2) | C16C—C15C—C6C | 118.5 (2) |
| C4B—C3B—C2B | 122.6 (2) | C21C—C16C—C17C | 119.3 (2) |
| C4B—C3B—H3BA | 118.7 | C21C—C16C—C15C | 118.7 (2) |
| C2B—C3B—H3BA | 118.7 | C17C—C16C—C15C | 122.0 (2) |
| C3B—C4B—C5B | 117.4 (2) | C18C—C17C—C16C | 120.1 (3) |
| C3B—C4B—C7B | 121.3 (2) | C18C—C17C—H17C | 120.0 |
| C5B—C4B—C7B | 121.3 (2) | C16C—C17C—H17C | 120.0 |
| C6B—C5B—C4B | 122.4 (2) | C17C—C18C—C19C | 120.3 (3) |
| C6B—C5B—H5BA | 118.8 | C17C—C18C—H18C | 119.8 |
| C4B—C5B—H5BA | 118.8 | C19C—C18C—H18C | 119.8 |
| C5B—C6B—C1B | 120.8 (2) | C18C—C19C—C20C | 119.6 (3) |
| C5B—C6B—C15B | 118.9 (2) | C18C—C19C—H19C | 120.2 |

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| C1B—C6B—C15B | 119.9 (2) | C20C—C19C—H19C | 120.2 |
| C4B—C7B—H7BA | 109.5 | C21C—C20C—C19C | 120.2 (3) |
| C4B—C7B—H7BB | 109.5 | C21C—C20C—H20C | 119.9 |
| H7BA—C7B—H7BB | 109.5 | C19C—C20C—H20C | 119.9 |
| C4B—C7B—H7BC | 109.5 | C20C—C21C—C16C | 120.5 (3) |
| H7BA—C7B—H7BC | 109.5 | C20C—C21C—H21C | 119.7 |
| H7BB—C7B—H7BC | 109.5 | C16C—C21C—H21C | 119.7 |
| O2B—C8B—C2B | 124.7 (2) | | |

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| O1B—Co—O1A—C1A | −172.3 (2) | C3B—C2B—C8B—C9B | 11.1 (3) |
| O2B—Co—O1A—C1A | 97.7 (2) | C1B—C2B—C8B—C9B | −170.4 (2) |
| O2C—Co—O1A—C1A | −84.0 (2) | O2B—C8B—C9B—C10B | −121.5 (2) |
| O2A—Co—O1A—C1A | 9.0 (2) | C2B—C8B—C9B—C10B | 57.5 (3) |
| O1C—Co—O2A—C8A | −179.2 (2) | O2B—C8B—C9B—C14B | 51.4 (3) |
| O1A—Co—O2A—C8A | 0.7 (2) | C2B—C8B—C9B—C14B | −129.7 (3) |
| O2B—Co—O2A—C8A | −88.7 (2) | C14B—C9B—C10B—C11B | −1.1 (4) |
| O2C—Co—O2A—C8A | 93.8 (2) | C8B—C9B—C10B—C11B | 171.7 (2) |
| Co—O1A—C1A—C2A | −5.2 (3) | C9B—C10B—C11B—C12B | 3.0 (4) |
| Co—O1A—C1A—C6A | 174.29 (16) | C10B—C11B—C12B—C13B | −1.8 (5) |
| O1A—C1A—C2A—C3A | 169.3 (2) | C11B—C12B—C13B—C14B | −1.3 (5) |
| C6A—C1A—C2A—C3A | −10.1 (3) | C12B—C13B—C14B—C9B | 3.1 (4) |
| O1A—C1A—C2A—C8A | −9.9 (4) | C10B—C9B—C14B—C13B | −1.9 (4) |
| C6A—C1A—C2A—C8A | 170.6 (2) | C8B—C9B—C14B—C13B | −174.8 (2) |
| C1A—C2A—C3A—C4A | 4.1 (4) | C5B—C6B—C15B—O3B | −46.5 (4) |
| C8A—C2A—C3A—C4A | −176.7 (2) | C1B—C6B—C15B—O3B | 126.7 (3) |
| C2A—C3A—C4A—C5A | 3.0 (4) | C5B—C6B—C15B—C16B | 129.9 (3) |
| C2A—C3A—C4A—C7A | −177.0 (2) | C1B—C6B—C15B—C16B | −56.9 (3) |
| C3A—C4A—C5A—C6A | −3.6 (4) | O3B—C15B—C16B—C17B | 160.0 (3) |
| C7A—C4A—C5A—C6A | 176.4 (2) | C6B—C15B—C16B—C17B | −16.3 (4) |
| C4A—C5A—C6A—C1A | −2.9 (4) | O3B—C15B—C16B—C21B | −14.6 (4) |
| C4A—C5A—C6A—C15A | −177.9 (2) | C6B—C15B—C16B—C21B | 169.1 (2) |
| O1A—C1A—C6A—C5A | −169.9 (2) | C21B—C16B—C17B—C18B | 2.5 (4) |
| C2A—C1A—C6A—C5A | 9.6 (3) | C15B—C16B—C17B—C18B | −172.0 (3) |
| O1A—C1A—C6A—C15A | 5.1 (3) | C16B—C17B—C18B—C19B | −1.3 (4) |
| C2A—C1A—C6A—C15A | −175.4 (2) | C17B—C18B—C19B—C20B | −1.0 (5) |
| Co—O2A—C8A—C2A | −13.9 (3) | C18B—C19B—C20B—C21B | 1.9 (4) |
| Co—O2A—C8A—C9A | 165.00 (15) | C19B—C20B—C21B—C16B | −0.6 (4) |
| C3A—C2A—C8A—O2A | −159.7 (2) | C17B—C16B—C21B—C20B | −1.6 (4) |
| C1A—C2A—C8A—O2A | 19.6 (3) | C15B—C16B—C21B—C20B | 173.2 (2) |
| C3A—C2A—C8A—C9A | 21.5 (3) | O1B—Co—O1C—C1C | 39.09 (17) |
| C1A—C2A—C8A—C9A | −159.2 (2) | O2B—Co—O1C—C1C | 129.11 (17) |
| O2A—C8A—C9A—C10A | 31.2 (3) | O2C—Co—O1C—C1C | −49.11 (17) |
| C2A—C8A—C9A—C10A | −149.9 (2) | O2A—Co—O1C—C1C | −142.14 (17) |
| O2A—C8A—C9A—C14A | −143.8 (2) | O1B—Co—O2C—C8C | −52.61 (19) |
| C2A—C8A—C9A—C14A | 35.1 (3) | O1C—Co—O2C—C8C | 37.41 (19) |
| C14A—C9A—C10A—C11A | −3.3 (4) | O1A—Co—O2C—C8C | −144.25 (19) |
| C8A—C9A—C10A—C11A | −178.5 (2) | O2A—Co—O2C—C8C | 127.12 (19) |
| C9A—C10A—C11A—C12A | 2.2 (4) | Co—O1C—C1C—C6C | −141.27 (18) |
| C10A—C11A—C12A—C13A | 0.4 (4) | Co—O1C—C1C—C2C | 37.7 (3) |

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| C11A—C12A—C13A—C14A | −1.8 (4) | O1C—C1C—C2C—C3C | −175.6 (2) |
| C12A—C13A—C14A—C9A | 0.6 (4) | C6C—C1C—C2C—C3C | 3.4 (3) |
| C10A—C9A—C14A—C13A | 1.9 (4) | O1C—C1C—C2C—C8C | 3.8 (4) |
| C8A—C9A—C14A—C13A | 176.8 (2) | C6C—C1C—C2C—C8C | −177.2 (2) |
| C5A—C6A—C15A—O3A | 36.1 (4) | C1C—C2C—C3C—C4C | −1.6 (4) |
| C1A—C6A—C15A—O3A | −139.0 (3) | C8C—C2C—C3C—C4C | 179.0 (2) |
| C5A—C6A—C15A—C16A | −141.4 (3) | C2C—C3C—C4C—C5C | −0.5 (4) |
| C1A—C6A—C15A—C16A | 43.6 (4) | C2C—C3C—C4C—C7C | 179.0 (3) |
| O3A—C15A—C16A—C17A | 31.6 (4) | C3C—C4C—C5C—C6C | 0.8 (4) |
| C6A—C15A—C16A—C17A | −150.9 (3) | C7C—C4C—C5C—C6C | −178.8 (3) |
| O3A—C15A—C16A—C21A | −145.5 (3) | C4C—C5C—C6C—C1C | 1.2 (4) |
| C6A—C15A—C16A—C21A | 31.9 (4) | C4C—C5C—C6C—C15C | 178.6 (2) |
| C21A—C16A—C17A—C18A | −1.0 (4) | O1C—C1C—C6C—C5C | 175.8 (2) |
| C15A—C16A—C17A—C18A | −178.2 (3) | C2C—C1C—C6C—C5C | −3.2 (4) |
| C16A—C17A—C18A—C19A | 2.0 (4) | O1C—C1C—C6C—C15C | −1.6 (3) |
| C17A—C18A—C19A—C20A | −1.3 (4) | C2C—C1C—C6C—C15C | 179.4 (2) |
| C18A—C19A—C20A—C21A | −0.5 (4) | Co—O2C—C8C—C2C | −10.6 (3) |
| C19A—C20A—C21A—C16A | 1.6 (4) | Co—O2C—C8C—C9C | 169.42 (15) |
| C17A—C16A—C21A—C20A | −0.8 (4) | C3C—C2C—C8C—O2C | 160.4 (2) |
| C15A—C16A—C21A—C20A | 176.3 (2) | C1C—C2C—C8C—O2C | −18.9 (4) |
| O1C—Co—O1B—C1B | 86.8 (2) | C3C—C2C—C8C—C9C | −19.5 (4) |
| O1A—Co—O1B—C1B | −93.0 (2) | C1C—C2C—C8C—C9C | 161.1 (2) |
| O2B—Co—O1B—C1B | −3.6 (2) | O2C—C8C—C9C—C14C | 145.7 (3) |
| O2C—Co—O1B—C1B | 173.8 (2) | C2C—C8C—C9C—C14C | −34.3 (4) |
| O1B—Co—O2B—C8B | 9.7 (2) | O2C—C8C—C9C—C10C | −32.4 (3) |
| O1C—Co—O2B—C8B | −80.2 (2) | C2C—C8C—C9C—C10C | 147.5 (2) |
| O1A—Co—O2B—C8B | 101.5 (2) | C14C—C9C—C10C—C11C | −0.4 (4) |
| O2A—Co—O2B—C8B | −170.1 (2) | C8C—C9C—C10C—C11C | 177.8 (2) |
| Co—O1B—C1B—C6B | −175.28 (16) | C9C—C10C—C11C—C12C | −0.4 (4) |
| Co—O1B—C1B—C2B | 1.2 (3) | C10C—C11C—C12C—C13C | 1.1 (5) |
| O1B—C1B—C2B—C3B | 176.5 (2) | C11C—C12C—C13C—C14C | −0.9 (5) |
| C6B—C1B—C2B—C3B | −7.0 (3) | C10C—C9C—C14C—C13C | 0.6 (4) |
| O1B—C1B—C2B—C8B | −2.1 (4) | C8C—C9C—C14C—C13C | −177.5 (3) |
| C6B—C1B—C2B—C8B | 174.5 (2) | C12C—C13C—C14C—C9C | 0.0 (5) |
| C1B—C2B—C3B—C4B | 2.8 (4) | C5C—C6C—C15C—O3C | 116.0 (3) |
| C8B—C2B—C3B—C4B | −178.7 (2) | C1C—C6C—C15C—O3C | −66.6 (3) |
| C2B—C3B—C4B—C5B | 3.3 (4) | C5C—C6C—C15C—C16C | −63.3 (3) |
| C2B—C3B—C4B—C7B | −178.4 (2) | C1C—C6C—C15C—C16C | 114.1 (3) |
| C3B—C4B—C5B—C6B | −5.1 (4) | O3C—C15C—C16C—C21C | −7.4 (4) |
| C7B—C4B—C5B—C6B | 176.6 (3) | C6C—C15C—C16C—C21C | 171.9 (2) |
| C4B—C5B—C6B—C1B | 0.6 (4) | O3C—C15C—C16C—C17C | 171.2 (2) |
| C4B—C5B—C6B—C15B | 173.7 (2) | C6C—C15C—C16C—C17C | −9.5 (3) |
| O1B—C1B—C6B—C5B | −177.8 (2) | C21C—C16C—C17C—C18C | 0.1 (4) |
| C2B—C1B—C6B—C5B | 5.4 (3) | C15C—C16C—C17C—C18C | −178.5 (2) |
| O1B—C1B—C6B—C15B | 9.2 (3) | C16C—C17C—C18C—C19C | 0.3 (4) |
| C2B—C1B—C6B—C15B | −167.6 (2) | C17C—C18C—C19C—C20C | −0.3 (5) |
| Co—O2B—C8B—C2B | −13.4 (3) | C18C—C19C—C20C—C21C | −0.1 (5) |
| Co—O2B—C8B—C9B | 165.51 (15) | C19C—C20C—C21C—C16C | 0.4 (4) |
| C3B—C2B—C8B—O2B | −170.1 (2) | C17C—C16C—C21C—C20C | −0.4 (4) |

| | | | |
|---|---|---|---|
| C1B—C2B—C8B—O2B | 8.4 (4) | C15C—C16C—C21C—C20C | 178.2 (2) |

*Hydrogen-bond geometry (Å, º)*

Cg7, Cg9, Cg11 and Cg12 are the centroids of the C9*A*–C14*A*, C9*C*–C14*C*, C16*B*–C21*B* and C16*C*–C21*C* rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12*A*—H12*A*···O2*B*$^{i}$ | 0.95 | 2.60 | 3.442 (3) | 147 |
| C13*A*—H13*A*···O3*C*$^{i}$ | 0.95 | 2.48 | 3.278 (3) | 141 |
| C13*B*—H13*B*···O3*B*$^{ii}$ | 0.95 | 2.39 | 3.311 (3) | 162 |
| C11*C*—H11*C*···O3*C*$^{iii}$ | 0.95 | 2.40 | 3.313 (3) | 161 |
| C10*B*—H10*B*···*Cg*12 | 0.95 | 2.70 | 3.634 (3) | 166 |
| C11*B*—H11*B*···*Cg*7$^{iv}$ | 0.95 | 2.72 | 3.479 (3) | 137 |
| C18*C*—H18*C*···*Cg*9$^{iv}$ | 0.95 | 2.99 | 3.720 (4) | 135 |
| C20*C*—H20*C*···*Cg*11$^{v}$ | 0.95 | 2.88 | 3.332 (3) | 110 |

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*, −*y*+3/2, *z*+1/2; (iii) −*x*+1, *y*+1/2, −*z*+1/2; (iv) *x*+1, *y*, *z*; (v) −*x*+2, *y*−1/2, −*z*+1/2.