# Dibenzo[*b*,*g*]indeno[1′,2′:3,4]fluoreno-[1,2-*d*]oxonine-5,11,16,21-tetraone

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The asymmetric unit of the title compound, $C_{34}H_{16}O_5$, contains two independent molecules (*A* and *B*) with similar conformations. The two benzene rings attached to the nine-membered ring are inclined to one another at 63.62 (14)° in molecule *A* and 68.23 (12)° in molecule *B*. One intramoleculer C—H⋯O hydrogen bond occurs in molecule *A* and two are observed in molecule *B*. In the crystal, molecules are linked by weak C—H⋯O hydrogen bonds, forming a three-dimensional network structure with $R_2^2(10)$ and $R_2^2(24)$ ring motifs. Aromatic $\pi$–$\pi$ stacking interactions [centroid–centroid distances = 3.7572 (19), 3.6996 (19) and 3.7043 (19) Å] are also observed. The unit cell contains a pair of voids of 37 (2) Å$^3$ about an inversion centre but the residual electron density (highest peak = 0.19 e Å$^{-3}$ and deepest hole = $-0.20$ e Å$^{-3}$) in the difference Fourier map suggests that no solvent molecule occupies this void.

## Related literature

1,3-Indandione undergoes self-condensation quite easily, see: Zargar & Khan (2012). For industrial and biological applications of indandion containing compounds see: Seniutinas *et al.* (2012); Jin *et al.* (2009). For ring conformations, see: Cremer & Pople (1975).
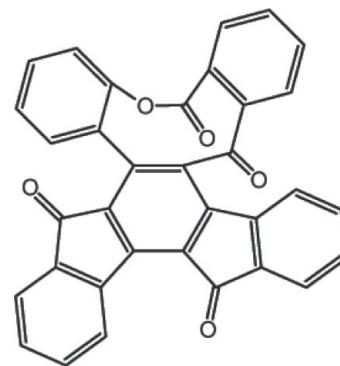
## Experimental

### Crystal data

| | |
|---|---|
| $C_{34}H_{16}O_5$ | $\gamma = 81.181\,(10)°$ |
| $M_r = 504.47$ | $V = 2382.5\,(12)$ Å$^3$ |
| Triclinic, $P\bar{1}$ | $Z = 4$ |
| $a = 12.230\,(4)$ Å | Mo $K\alpha$ radiation |
| $b = 12.346\,(3)$ Å | $\mu = 0.10$ mm$^{-1}$ |
| $c = 16.794\,(5)$ Å | $T = 296$ K |
| $\alpha = 82.229\,(7)°$ | $0.28 \times 0.18 \times 0.14$ mm |
| $\beta = 72.773\,(6)°$ | |

### Data collection

| | |
|---|---|
| Bruker Kappa APEXII CCD diffractometer | 38137 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2005) | 10895 independent reflections |
| | 4858 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.980$, $T_{max} = 0.987$ | $R_{int} = 0.061$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.056$ | 704 parameters |
| $wR(F^2) = 0.135$ | H-atom parameters constrained |
| $S = 0.94$ | $\Delta\rho_{max} = 0.19$ e Å$^{-3}$ |
| 10895 reflections | $\Delta\rho_{min} = -0.21$ e Å$^{-3}$ |

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C24—H24⋯O10[i] | 0.93 | 2.56 | 3.302 (3) | 137 |
| C30—H30⋯O5[ii] | 0.93 | 2.60 | 3.507 (3) | 166 |
| C32—H32⋯O7[iii] | 0.93 | 2.49 | 3.398 (3) | 166 |
| C33—H33⋯O4 | 0.93 | 2.32 | 3.087 (3) | 139 |
| C39—H39⋯O1[iv] | 0.93 | 2.36 | 3.115 (3) | 139 |
| C56—H56⋯O8 | 0.93 | 2.52 | 3.210 (3) | 131 |
| C58—H58⋯O7[v] | 0.93 | 2.52 | 3.377 (3) | 154 |
| C67—H67⋯O9 | 0.93 | 2.36 | 3.117 (3) | 139 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

# organic compounds

University and the University of Sargodha for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5643).

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# supporting information

## Dibenzo[*b,g*]indeno[1′,2′:3,4]fluoreno[1,2-*d*]oxonine-5,11,16,21-tetraone

**Shaaban Kamel Mohamed, Mehmet Akkurt, Muhammad N. Tahir, Antar A. Abdelhamid and Adel A. Marzouk**

### S1. Comment

1,3-indandione is an important member of class of 1,3-diketo compounds. It is a very strong C-nucleophile. It undergoes self-condensation quite easily, resulting in a dimer *e.g.* bindone and trimer (Zargar & Khan, 2012). Due to such unusual chemical reactivity, 1,3-indandione showed a wide range of industrial and pharmaceutical applications. It is a founder structure in most of non linear optical (NLO) compounds, chromophores (Seniutinas *et al.*, 2012) and pesticide molecules such as diphacinone, chlorophacinone, valone, and Pindone (Jin *et al.*, 2009). Such facts prompted us to synthesize and study the crystal determination of the title compound (I).

Figures 1 and 2 show two enantiomeric molecules (A with O1 and B with O6) of the title compound in the asymmetric unit. The values of the geometric parameters of both molecules A and B are similar with each other. In molecule A, the two benzene rings (C1–C6 and C8–C13) which are attached to the nine-membered ring are inclined to one another by 63.62 (14)°, and in molecule B, the two benzene rings (C35–C40 and C42–C47) by 68.23 (12)°.

In molecule A, the puckering parameters for the nine-membered ring (O1/C1/C6—C8/C13—C16) are $Q(2) = 1.880\ (3)$ Å, $\varphi\ (2) = 58.83\ (8)°$; $Q(3) = 0.189\ (2)$ Å, $\varphi\ (3) = 10.2\ (8)°$; $Q(4) = 0.118\ (3)$ Å, $\varphi\ (4) = 136.5\ (12)°$ and $Q_T$ (total puckering amplitude) = 1.893 (3) Å (Cremer & Pople, 1975). In molecule B, the puckering parameters for the nine-membered ring (O6/C35/C40—C42/C47—C50) are $Q(2) = 1.864\ (3)$ Å, $\varphi\ (2) = 246.61\ (7)°$; $Q(3) = 0.223\ (2)$ Å, $\varphi\ (3) = 177.7\ (7)°$; $Q(4) = 0.143\ (2)$ Å, $\varphi\ (4) = 313.4\ (10)°$ and $Q_T$ (total puckering amplitude) = 1.882 (3) Å.

In the crystal, C—H⋯O hydrogen bonds link the A and B molecules (Fig. 3, Table 1). The crystal packing is stabilized by additional three π–π stacking interactions [*Cg*5⋯*Cg*31 (*x*, *y*, *z*) = 3.7572 (19) Å, *Cg*7⋯*Cg*32(-1 + *x*, *y*, *z*) = 3.6996 (19) Å and *Cg*31⋯*Cg*31(1 - *x*, -*y*, 2 - *z*) = 3.7043 (19) Å; where *Cg*5, *Cg*7, *Cg*31 and *Cg*32 are the centroids of the C15–C20, C29–C34, C55–C60 and C63–C68 rings, respectively].

### S2. Experimental

The title compound was obtained from a reaction mixture of 4 mmol (576 mg) indandione and 2 mmol (244 mg) salicyl-aldehyde in presence of 1 mmol (90 mg) 1,3-diaminopropan-2-ol in 50 ml e thanol. The reaction mixture was refluxed for 6 h at 350 K. The excess solvent was evaporated under vacum and the obtained solid was recrystallized from acetic acid to afford a good yield (82%) of dark green crystals (m.p. 575 K) suitable for X-ray diffraction.

### S3. Refinement

All H atoms were located geometrically and treated as riding atoms with C—H = 0.93 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$.
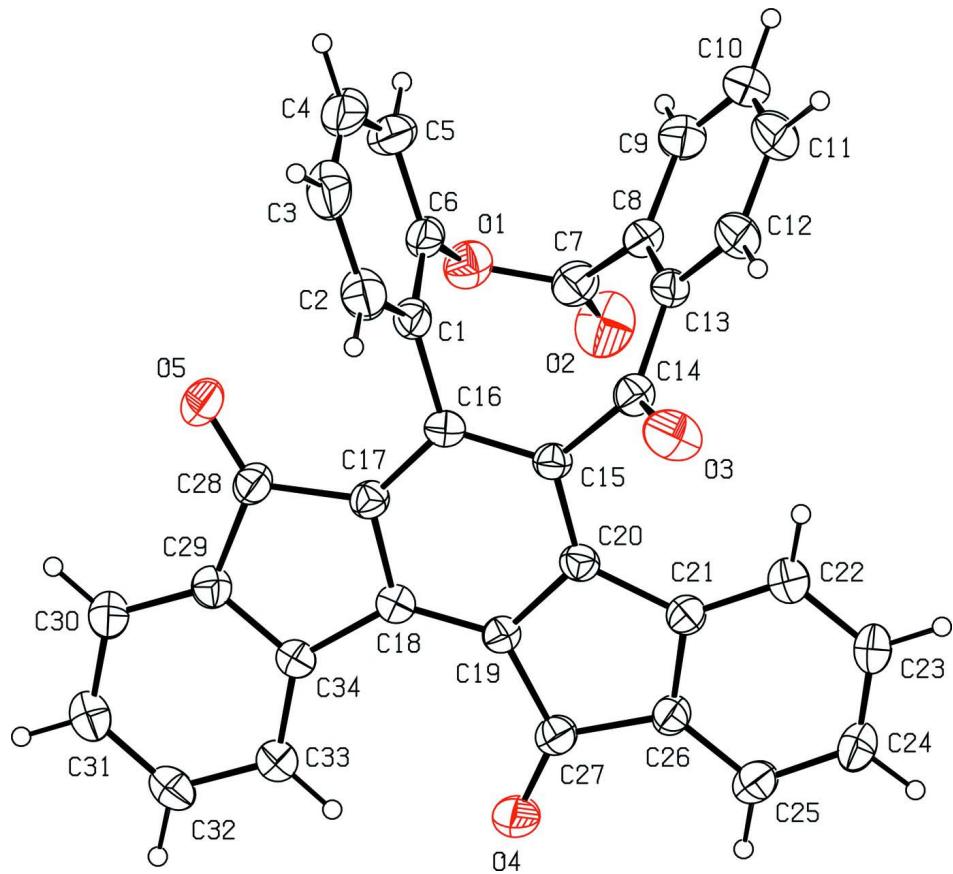
**Figure 1**

View of the molecule A of two molecules of (I) in the asymmetric unit. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.
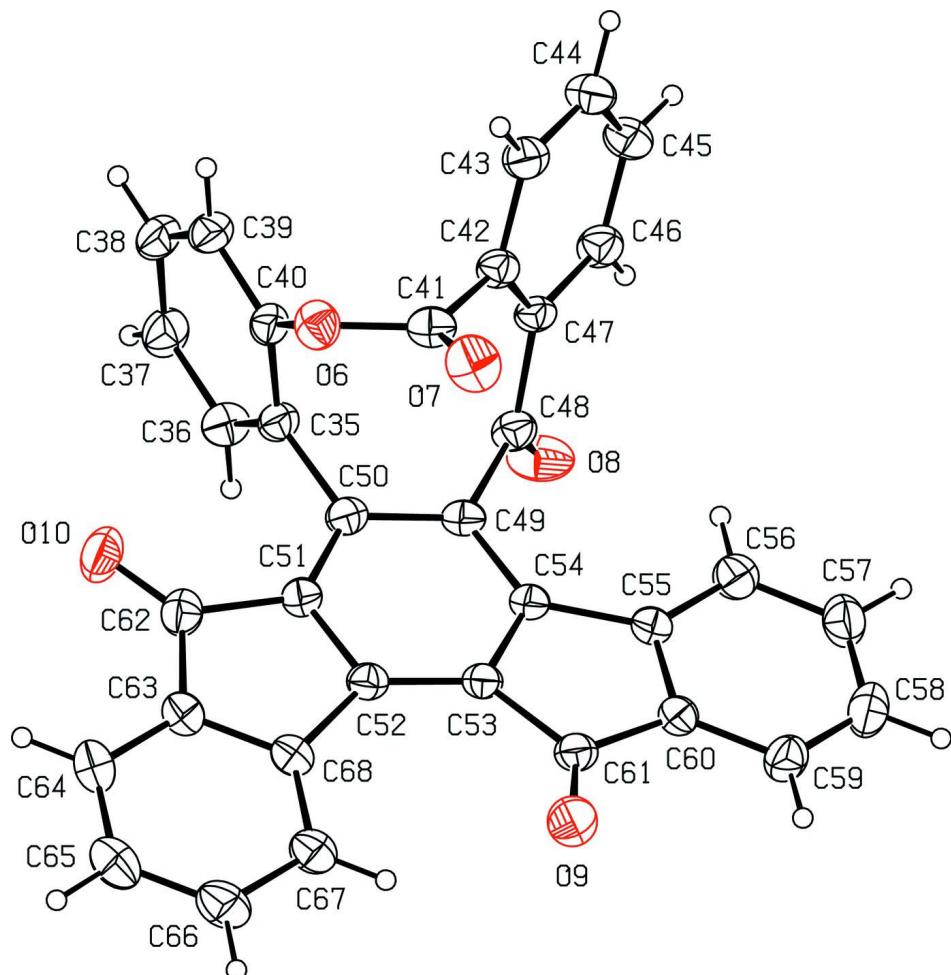
**Figure 2**
View of the molecule B of two molecules of (I) in the asymmetric unit. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.
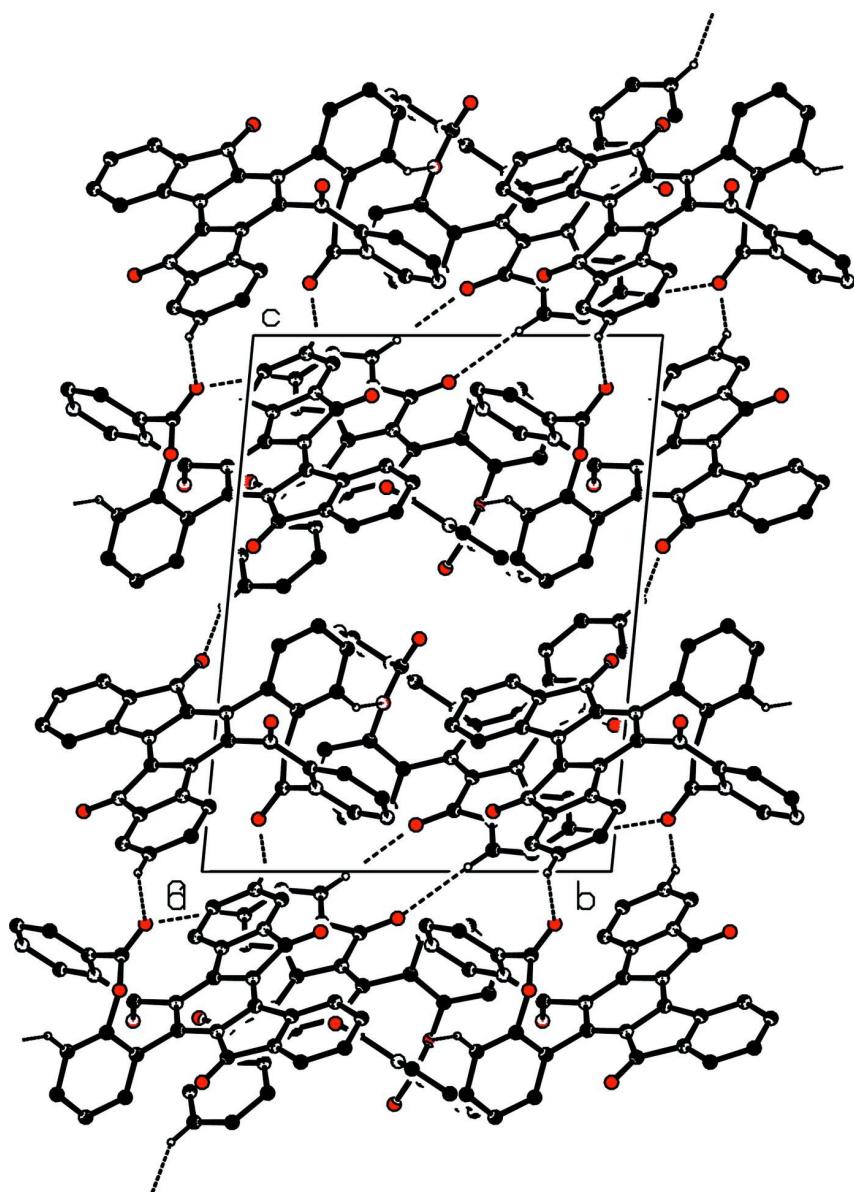
**Figure 3**

View of the molecular packing of (I) down the *a* axis. H atoms not involved in hydrogen bonding have been omitted for clarity.

**(I)**

*Crystal data*

| | |
|---|---|
| C₃₄H₁₆O₅ | $\gamma = 81.181\ (10)°$ |
| $M_r = 504.47$ | $V = 2382.5\ (12)\ \text{Å}^3$ |
| Triclinic, $P\bar{1}$ | $Z = 4$ |
| Hall symbol: -P 1 | $F(000) = 1040$ |
| $a = 12.230\ (4)\ \text{Å}$ | $D_x = 1.406\ \text{Mg m}^{-3}$ |
| $b = 12.346\ (3)\ \text{Å}$ | Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{Å}$ |
| $c = 16.794\ (5)\ \text{Å}$ | Cell parameters from 182 reflections |
| $\alpha = 82.229\ (7)°$ | $\theta = 3.3–21.5°$ |
| $\beta = 72.773\ (6)°$ | $\mu = 0.10\ \text{mm}^{-1}$ |

$T$ = 296 K

Prism, dark green

0.28 × 0.18 × 0.14 mm

*Data collection*

| | |
|---|---|
| Bruker Kappa APEXII CCD diffractometer | 38137 measured reflections |
| Radiation source: fine-focus sealed tube | 10895 independent reflections |
| Graphite monochromator | 4858 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 0.81 pixels mm$^{-1}$ | $R_{int}$ = 0.061 |
| $\omega$ scans | $\theta_{max}$ = 27.6°, $\theta_{min}$ = 2.3° |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2005) | $h = -15{\rightarrow}15$ |
| | $k = -16{\rightarrow}16$ |
| $T_{min}$ = 0.980, $T_{max}$ = 0.987 | $l = -21{\rightarrow}21$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.056 | $w = 1/[\sigma^2(F_o^2) + (0.0501P)^2]$ |
| $wR(F^2)$ = 0.135 | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 0.94 | $(\Delta/\sigma)_{max} < 0.001$ |
| 10895 reflections | $\Delta\rho_{max}$ = 0.19 e Å$^{-3}$ |
| 704 parameters | $\Delta\rho_{min}$ = −0.21 e Å$^{-3}$ |
| 0 restraints | Extinction correction: *SHELXL97* (Sheldrick, 2008), FC$^*$=KFC[1+0.001XFC$^2\Lambda^3$/SIN(2Θ)]$^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.0020 (4) |
| Secondary atom site location: difference Fourier map | |

*Special details*

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

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted $R$-factors $wR$ and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -$R$-factor-obs *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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.30343 (13) | 0.59668 (14) | 0.68545 (12) | 0.0606 (7) |
| O2 | 0.36189 (17) | 0.52360 (19) | 0.56612 (14) | 0.0919 (10) |
| O3 | 0.65201 (14) | 0.36139 (15) | 0.71664 (13) | 0.0755 (8) |
| O4 | 0.31239 (15) | 0.02705 (15) | 0.72691 (12) | 0.0721 (8) |
| O5 | 0.12537 (14) | 0.48837 (16) | 0.91275 (12) | 0.0710 (8) |
| C1 | 0.36124 (18) | 0.5327 (2) | 0.80850 (17) | 0.0457 (9) |
| C2 | 0.3815 (2) | 0.5551 (3) | 0.88099 (18) | 0.0660 (11) |
| C3 | 0.3712 (2) | 0.6644 (3) | 0.8990 (2) | 0.0826 (16) |
| C4 | 0.3414 (2) | 0.7490 (3) | 0.8436 (3) | 0.0847 (16) |
| C5 | 0.3211 (2) | 0.7288 (2) | 0.7722 (2) | 0.0709 (13) |
| C6 | 0.33166 (19) | 0.6210 (2) | 0.75593 (17) | 0.0495 (10) |
| C7 | 0.3894 (2) | 0.5616 (2) | 0.61735 (19) | 0.0570 (11) |

| C8 | 0.5070 (2) | 0.5881 (2) | 0.61130 (15) | 0.0474 (9) |
|---|---|---|---|---|
| C9 | 0.5342 (3) | 0.6868 (2) | 0.56465 (18) | 0.0692 (12) |
| C10 | 0.6393 (3) | 0.7211 (3) | 0.5530 (2) | 0.0821 (14) |
| C11 | 0.7199 (3) | 0.6572 (3) | 0.5856 (2) | 0.0797 (15) |
| C12 | 0.6954 (2) | 0.5587 (2) | 0.63184 (18) | 0.0616 (11) |
| C13 | 0.58751 (19) | 0.5234 (2) | 0.64604 (15) | 0.0431 (9) |
| C14 | 0.57028 (19) | 0.4167 (2) | 0.69716 (16) | 0.0462 (9) |
| C15 | 0.45753 (17) | 0.36805 (19) | 0.72787 (14) | 0.0400 (9) |
| C16 | 0.36222 (19) | 0.41890 (19) | 0.78720 (15) | 0.0422 (9) |
| C17 | 0.26743 (18) | 0.3624 (2) | 0.82399 (14) | 0.0415 (9) |
| C18 | 0.26223 (18) | 0.2556 (2) | 0.80507 (14) | 0.0407 (8) |
| C19 | 0.35423 (18) | 0.20753 (19) | 0.74519 (14) | 0.0403 (8) |
| C20 | 0.45172 (18) | 0.2643 (2) | 0.70666 (15) | 0.0416 (9) |
| C21 | 0.53516 (18) | 0.1954 (2) | 0.64342 (15) | 0.0445 (9) |
| C22 | 0.6417 (2) | 0.2118 (2) | 0.58698 (17) | 0.0609 (10) |
| C23 | 0.6949 (2) | 0.1317 (2) | 0.53227 (18) | 0.0672 (11) |
| C24 | 0.6467 (2) | 0.0389 (2) | 0.53273 (18) | 0.0659 (11) |
| C25 | 0.5414 (2) | 0.0214 (2) | 0.58938 (17) | 0.0585 (10) |
| C26 | 0.48748 (19) | 0.1004 (2) | 0.64358 (15) | 0.0449 (9) |
| C27 | 0.3741 (2) | 0.0999 (2) | 0.70820 (16) | 0.0482 (10) |
| C28 | 0.1557 (2) | 0.3987 (2) | 0.88562 (16) | 0.0477 (9) |
| C29 | 0.08788 (19) | 0.3041 (2) | 0.90507 (15) | 0.0456 (9) |
| C30 | −0.02000 (19) | 0.2945 (2) | 0.95961 (16) | 0.0532 (10) |
| C31 | −0.0662 (2) | 0.1982 (2) | 0.96602 (17) | 0.0588 (10) |
| C32 | −0.0065 (2) | 0.1132 (2) | 0.91909 (16) | 0.0556 (10) |
| C33 | 0.10298 (19) | 0.1220 (2) | 0.86364 (15) | 0.0503 (9) |
| C34 | 0.15016 (18) | 0.2189 (2) | 0.85727 (15) | 0.0417 (9) |
| O6 | 1.00908 (13) | −0.17362 (14) | 0.77863 (11) | 0.0535 (7) |
| O7 | 0.90062 (15) | −0.12612 (16) | 0.90231 (12) | 0.0674 (8) |
| O8 | 0.63534 (16) | −0.13362 (14) | 0.72125 (13) | 0.0714 (8) |
| O9 | 0.68213 (15) | 0.30354 (15) | 0.88768 (11) | 0.0639 (7) |
| O10 | 1.11392 (14) | 0.04935 (15) | 0.60688 (12) | 0.0679 (7) |
| C35 | 0.94112 (18) | −0.11759 (19) | 0.65889 (16) | 0.0419 (9) |
| C36 | 0.9417 (2) | −0.1352 (2) | 0.57890 (17) | 0.0529 (10) |
| C37 | 1.0053 (2) | −0.2271 (2) | 0.54203 (17) | 0.0577 (10) |
| C38 | 1.0671 (2) | −0.3024 (2) | 0.5844 (2) | 0.0609 (10) |
| C39 | 1.06743 (19) | −0.2873 (2) | 0.66449 (19) | 0.0557 (10) |
| C40 | 1.00473 (18) | −0.1955 (2) | 0.69976 (16) | 0.0433 (9) |
| C41 | 0.9114 (2) | −0.1772 (2) | 0.84396 (18) | 0.0483 (10) |
| C42 | 0.83080 (18) | −0.25756 (19) | 0.84404 (15) | 0.0409 (8) |
| C43 | 0.8502 (2) | −0.3585 (2) | 0.88940 (15) | 0.0504 (10) |
| C44 | 0.7807 (2) | −0.4394 (2) | 0.89913 (17) | 0.0586 (11) |
| C45 | 0.6915 (2) | −0.4225 (2) | 0.86307 (17) | 0.0573 (10) |
| C46 | 0.67236 (19) | −0.3245 (2) | 0.81736 (16) | 0.0498 (10) |
| C47 | 0.74017 (18) | −0.23984 (19) | 0.80699 (14) | 0.0389 (8) |
| C48 | 0.70772 (19) | −0.1365 (2) | 0.75803 (16) | 0.0453 (9) |
| C49 | 0.76039 (18) | −0.03298 (19) | 0.75539 (15) | 0.0407 (8) |
| C50 | 0.87355 (18) | −0.02196 (19) | 0.70404 (14) | 0.0408 (8) |

| | | | |
|---|---|---|---|
| C51 | 0.91980 (18) | 0.0738 (2) | 0.70171 (14) | 0.0411 (8) |
| C52 | 0.85951 (18) | 0.16119 (19) | 0.74945 (14) | 0.0391 (8) |
| C53 | 0.74977 (18) | 0.14884 (18) | 0.80130 (14) | 0.0384 (8) |
| C54 | 0.69851 (18) | 0.05350 (19) | 0.80181 (14) | 0.0383 (8) |
| C55 | 0.57903 (18) | 0.0654 (2) | 0.85817 (15) | 0.0416 (8) |
| C56 | 0.49093 (19) | −0.0013 (2) | 0.87878 (16) | 0.0531 (10) |
| C57 | 0.3861 (2) | 0.0352 (2) | 0.93379 (17) | 0.0606 (11) |
| C58 | 0.3681 (2) | 0.1337 (3) | 0.96666 (17) | 0.0616 (10) |
| C59 | 0.4552 (2) | 0.2002 (2) | 0.94781 (15) | 0.0542 (10) |
| C60 | 0.55958 (19) | 0.1651 (2) | 0.89297 (15) | 0.0433 (9) |
| C61 | 0.66597 (19) | 0.2206 (2) | 0.86300 (15) | 0.0443 (9) |
| C62 | 1.0373 (2) | 0.1048 (2) | 0.65342 (16) | 0.0490 (10) |
| C63 | 1.03846 (19) | 0.2175 (2) | 0.67471 (15) | 0.0456 (9) |
| C64 | 1.1243 (2) | 0.2854 (2) | 0.64486 (16) | 0.0558 (10) |
| C65 | 1.1039 (2) | 0.3894 (3) | 0.67096 (18) | 0.0656 (11) |
| C66 | 0.9996 (2) | 0.4235 (2) | 0.72629 (18) | 0.0645 (11) |
| C67 | 0.9133 (2) | 0.3553 (2) | 0.75702 (16) | 0.0538 (10) |
| C68 | 0.93334 (19) | 0.2515 (2) | 0.73056 (15) | 0.0418 (9) |
| H2 | 0.40190 | 0.49770 | 0.91780 | 0.0790* |
| H3 | 0.38440 | 0.68000 | 0.94780 | 0.0990* |
| H4 | 0.33520 | 0.82140 | 0.85550 | 0.1020* |
| H5 | 0.30060 | 0.78610 | 0.73540 | 0.0850* |
| H9 | 0.48030 | 0.73010 | 0.54110 | 0.0830* |
| H10 | 0.65600 | 0.78820 | 0.52260 | 0.0980* |
| H11 | 0.79180 | 0.68040 | 0.57660 | 0.0960* |
| H12 | 0.75090 | 0.51540 | 0.65370 | 0.0740* |
| H22 | 0.67620 | 0.27430 | 0.58580 | 0.0730* |
| H23 | 0.76600 | 0.14180 | 0.49400 | 0.0810* |
| H24 | 0.68460 | −0.01250 | 0.49500 | 0.0790* |
| H25 | 0.50800 | −0.04180 | 0.59090 | 0.0700* |
| H30 | −0.06040 | 0.35170 | 0.99120 | 0.0640* |
| H31 | −0.13900 | 0.19010 | 1.00250 | 0.0710* |
| H32 | −0.03970 | 0.04870 | 0.92450 | 0.0670* |
| H33 | 0.14290 | 0.06460 | 0.83200 | 0.0600* |
| H36 | 0.89900 | −0.08480 | 0.54990 | 0.0630* |
| H37 | 1.00590 | −0.23780 | 0.48810 | 0.0690* |
| H38 | 1.10920 | −0.36430 | 0.55920 | 0.0730* |
| H39 | 1.10930 | −0.33840 | 0.69360 | 0.0670* |
| H43 | 0.91110 | −0.37100 | 0.91330 | 0.0610* |
| H44 | 0.79390 | −0.50580 | 0.93020 | 0.0700* |
| H45 | 0.64430 | −0.47730 | 0.86970 | 0.0690* |
| H46 | 0.61240 | −0.31420 | 0.79250 | 0.0600* |
| H56 | 0.50180 | −0.06840 | 0.85640 | 0.0640* |
| H57 | 0.32650 | −0.00880 | 0.94860 | 0.0730* |
| H58 | 0.29630 | 0.15630 | 1.00220 | 0.0740* |
| H59 | 0.44400 | 0.26650 | 0.97130 | 0.0650* |
| H64 | 1.19450 | 0.26140 | 0.60790 | 0.0670* |
| H65 | 1.16040 | 0.43670 | 0.65130 | 0.0790* |

| | | | | | |
|---|---|---|---|---|---|
| H66 | 0.98690 | 0.49400 | 0.74340 | 0.0770* | |
| H67 | 0.84370 | 0.37910 | 0.79460 | 0.0650* | |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0502 (10) | 0.0595 (13) | 0.0732 (14) | 0.0036 (9) | −0.0241 (10) | −0.0066 (11) |
| O2 | 0.0874 (15) | 0.120 (2) | 0.0876 (17) | −0.0121 (13) | −0.0433 (13) | −0.0343 (15) |
| O3 | 0.0540 (11) | 0.0714 (14) | 0.1047 (17) | −0.0081 (10) | −0.0386 (11) | 0.0168 (12) |
| O4 | 0.0663 (12) | 0.0524 (13) | 0.0930 (16) | −0.0217 (10) | −0.0010 (11) | −0.0229 (11) |
| O5 | 0.0637 (11) | 0.0605 (14) | 0.0801 (15) | −0.0056 (10) | 0.0023 (10) | −0.0303 (12) |
| C1 | 0.0398 (13) | 0.0489 (18) | 0.0484 (17) | −0.0110 (12) | −0.0061 (12) | −0.0121 (15) |
| C2 | 0.0640 (17) | 0.079 (2) | 0.058 (2) | −0.0239 (16) | −0.0094 (15) | −0.0167 (18) |
| C3 | 0.074 (2) | 0.108 (3) | 0.071 (3) | −0.039 (2) | 0.0024 (18) | −0.046 (2) |
| C4 | 0.066 (2) | 0.070 (3) | 0.113 (3) | −0.0272 (18) | 0.009 (2) | −0.047 (3) |
| C5 | 0.0593 (18) | 0.045 (2) | 0.103 (3) | −0.0059 (14) | −0.0089 (18) | −0.0208 (19) |
| C6 | 0.0387 (13) | 0.0469 (19) | 0.060 (2) | −0.0056 (12) | −0.0047 (13) | −0.0153 (16) |
| C7 | 0.0576 (17) | 0.0535 (19) | 0.060 (2) | 0.0011 (14) | −0.0209 (16) | −0.0051 (16) |
| C8 | 0.0522 (15) | 0.0397 (17) | 0.0469 (17) | −0.0037 (13) | −0.0083 (13) | −0.0073 (14) |
| C9 | 0.078 (2) | 0.052 (2) | 0.065 (2) | −0.0009 (16) | −0.0078 (17) | 0.0024 (17) |
| C10 | 0.092 (2) | 0.048 (2) | 0.083 (3) | −0.0186 (19) | 0.014 (2) | −0.0023 (18) |
| C11 | 0.0650 (19) | 0.076 (3) | 0.090 (3) | −0.0323 (18) | 0.0043 (18) | −0.012 (2) |
| C12 | 0.0518 (16) | 0.063 (2) | 0.069 (2) | −0.0189 (14) | −0.0096 (14) | −0.0059 (17) |
| C13 | 0.0436 (13) | 0.0426 (16) | 0.0430 (16) | −0.0102 (12) | −0.0084 (12) | −0.0071 (13) |
| C14 | 0.0397 (13) | 0.0490 (17) | 0.0516 (17) | −0.0043 (12) | −0.0153 (12) | −0.0067 (14) |
| C15 | 0.0401 (13) | 0.0363 (16) | 0.0442 (16) | −0.0060 (11) | −0.0122 (12) | −0.0037 (13) |
| C16 | 0.0449 (13) | 0.0376 (16) | 0.0455 (16) | −0.0076 (11) | −0.0138 (12) | −0.0031 (13) |
| C17 | 0.0419 (13) | 0.0399 (16) | 0.0440 (16) | −0.0050 (11) | −0.0125 (12) | −0.0079 (13) |
| C18 | 0.0410 (13) | 0.0414 (16) | 0.0409 (15) | −0.0057 (11) | −0.0132 (12) | −0.0031 (13) |
| C19 | 0.0428 (13) | 0.0373 (16) | 0.0404 (15) | −0.0049 (11) | −0.0105 (12) | −0.0054 (12) |
| C20 | 0.0425 (13) | 0.0378 (16) | 0.0435 (16) | −0.0050 (11) | −0.0124 (12) | 0.0006 (13) |
| C21 | 0.0409 (13) | 0.0420 (17) | 0.0479 (17) | −0.0008 (12) | −0.0112 (12) | −0.0022 (13) |
| C22 | 0.0512 (15) | 0.0572 (19) | 0.066 (2) | −0.0088 (14) | −0.0021 (15) | −0.0073 (16) |
| C23 | 0.0484 (15) | 0.066 (2) | 0.071 (2) | −0.0019 (15) | 0.0081 (15) | −0.0130 (18) |
| C24 | 0.0563 (17) | 0.062 (2) | 0.065 (2) | 0.0077 (15) | 0.0011 (15) | −0.0147 (17) |
| C25 | 0.0583 (16) | 0.0475 (18) | 0.067 (2) | 0.0006 (13) | −0.0134 (15) | −0.0134 (16) |
| C26 | 0.0454 (13) | 0.0424 (17) | 0.0434 (16) | 0.0007 (12) | −0.0094 (12) | −0.0061 (13) |
| C27 | 0.0484 (14) | 0.0433 (18) | 0.0525 (18) | −0.0041 (13) | −0.0125 (13) | −0.0087 (14) |
| C28 | 0.0477 (14) | 0.0460 (18) | 0.0477 (17) | −0.0008 (13) | −0.0096 (12) | −0.0126 (14) |
| C29 | 0.0430 (13) | 0.0502 (18) | 0.0448 (16) | −0.0072 (12) | −0.0126 (12) | −0.0059 (14) |
| C30 | 0.0469 (15) | 0.062 (2) | 0.0496 (18) | −0.0067 (13) | −0.0094 (13) | −0.0110 (15) |
| C31 | 0.0500 (15) | 0.071 (2) | 0.0520 (19) | −0.0132 (15) | −0.0069 (13) | −0.0040 (16) |
| C32 | 0.0579 (16) | 0.059 (2) | 0.0522 (18) | −0.0233 (14) | −0.0149 (14) | 0.0039 (15) |
| C33 | 0.0492 (14) | 0.0487 (18) | 0.0512 (17) | −0.0084 (13) | −0.0101 (13) | −0.0046 (14) |
| C34 | 0.0432 (13) | 0.0412 (16) | 0.0413 (16) | −0.0084 (12) | −0.0123 (12) | −0.0014 (13) |
| O6 | 0.0445 (10) | 0.0616 (13) | 0.0568 (12) | −0.0101 (8) | −0.0177 (9) | −0.0017 (10) |
| O7 | 0.0801 (13) | 0.0696 (14) | 0.0628 (14) | −0.0236 (10) | −0.0230 (11) | −0.0188 (11) |
| O8 | 0.0838 (13) | 0.0526 (13) | 0.0974 (16) | −0.0077 (10) | −0.0588 (12) | −0.0003 (11) |

| | | | | | |
|---|---|---|---|---|---|
| O9 | 0.0766 (12) | 0.0522 (13) | 0.0598 (13) | −0.0122 (10) | −0.0051 (10) | −0.0212 (10) |
| O10 | 0.0512 (10) | 0.0734 (14) | 0.0675 (14) | −0.0011 (10) | 0.0048 (10) | −0.0224 (11) |
| C35 | 0.0390 (12) | 0.0360 (16) | 0.0491 (17) | −0.0022 (11) | −0.0097 (12) | −0.0078 (13) |
| C36 | 0.0554 (15) | 0.0476 (18) | 0.0556 (19) | −0.0014 (13) | −0.0173 (14) | −0.0066 (15) |
| C37 | 0.0607 (16) | 0.056 (2) | 0.0534 (18) | −0.0045 (14) | −0.0071 (14) | −0.0182 (16) |
| C38 | 0.0513 (16) | 0.0441 (18) | 0.076 (2) | 0.0000 (13) | 0.0015 (15) | −0.0173 (17) |
| C39 | 0.0391 (13) | 0.0434 (18) | 0.078 (2) | 0.0013 (12) | −0.0110 (14) | −0.0025 (16) |
| C40 | 0.0349 (12) | 0.0421 (17) | 0.0497 (17) | −0.0046 (11) | −0.0065 (12) | −0.0061 (14) |
| C41 | 0.0534 (16) | 0.0418 (17) | 0.0538 (19) | −0.0029 (13) | −0.0230 (15) | −0.0035 (15) |
| C42 | 0.0463 (13) | 0.0345 (15) | 0.0429 (16) | −0.0040 (11) | −0.0125 (12) | −0.0085 (13) |
| C43 | 0.0541 (15) | 0.0461 (18) | 0.0496 (17) | 0.0006 (13) | −0.0155 (13) | −0.0048 (14) |
| C44 | 0.0695 (18) | 0.0395 (18) | 0.062 (2) | −0.0041 (14) | −0.0153 (15) | 0.0013 (15) |
| C45 | 0.0615 (16) | 0.0373 (18) | 0.073 (2) | −0.0146 (13) | −0.0149 (15) | −0.0038 (15) |
| C46 | 0.0473 (14) | 0.0411 (17) | 0.0625 (19) | −0.0057 (12) | −0.0148 (13) | −0.0107 (14) |
| C47 | 0.0434 (13) | 0.0293 (14) | 0.0438 (15) | −0.0015 (11) | −0.0114 (11) | −0.0085 (12) |
| C48 | 0.0449 (14) | 0.0388 (17) | 0.0537 (17) | −0.0023 (12) | −0.0152 (13) | −0.0092 (13) |
| C49 | 0.0447 (13) | 0.0330 (15) | 0.0452 (16) | −0.0010 (11) | −0.0173 (12) | 0.0001 (12) |
| C50 | 0.0447 (13) | 0.0365 (16) | 0.0402 (15) | 0.0008 (12) | −0.0126 (12) | −0.0047 (12) |
| C51 | 0.0396 (13) | 0.0398 (16) | 0.0417 (15) | −0.0017 (12) | −0.0107 (11) | −0.0012 (13) |
| C52 | 0.0446 (13) | 0.0345 (15) | 0.0378 (15) | −0.0021 (11) | −0.0132 (12) | −0.0017 (12) |
| C53 | 0.0441 (13) | 0.0302 (15) | 0.0385 (15) | −0.0020 (11) | −0.0099 (11) | −0.0018 (12) |
| C54 | 0.0410 (12) | 0.0326 (15) | 0.0391 (15) | −0.0015 (11) | −0.0110 (11) | 0.0005 (12) |
| C55 | 0.0433 (13) | 0.0377 (16) | 0.0411 (15) | −0.0033 (12) | −0.0116 (11) | 0.0031 (13) |
| C56 | 0.0494 (15) | 0.0491 (18) | 0.0607 (19) | −0.0084 (13) | −0.0141 (14) | −0.0049 (14) |
| C57 | 0.0477 (16) | 0.069 (2) | 0.060 (2) | −0.0134 (14) | −0.0068 (14) | 0.0000 (17) |
| C58 | 0.0437 (15) | 0.081 (2) | 0.0511 (19) | 0.0006 (15) | −0.0039 (13) | −0.0053 (17) |
| C59 | 0.0556 (16) | 0.0553 (19) | 0.0451 (17) | 0.0032 (14) | −0.0065 (13) | −0.0103 (14) |
| C60 | 0.0468 (14) | 0.0416 (17) | 0.0359 (15) | −0.0014 (12) | −0.0077 (12) | 0.0020 (13) |
| C61 | 0.0544 (15) | 0.0363 (16) | 0.0381 (16) | 0.0004 (12) | −0.0098 (12) | −0.0035 (13) |
| C62 | 0.0439 (14) | 0.0572 (19) | 0.0432 (17) | −0.0035 (13) | −0.0097 (13) | −0.0041 (14) |
| C63 | 0.0490 (15) | 0.0465 (17) | 0.0412 (16) | −0.0106 (13) | −0.0118 (12) | −0.0005 (13) |
| C64 | 0.0530 (15) | 0.067 (2) | 0.0444 (17) | −0.0185 (15) | −0.0061 (13) | 0.0002 (15) |
| C65 | 0.0689 (19) | 0.063 (2) | 0.067 (2) | −0.0283 (16) | −0.0184 (17) | 0.0078 (17) |
| C66 | 0.079 (2) | 0.0478 (19) | 0.072 (2) | −0.0239 (16) | −0.0221 (18) | −0.0035 (16) |
| C67 | 0.0564 (15) | 0.0445 (18) | 0.0618 (19) | −0.0145 (13) | −0.0151 (14) | −0.0030 (15) |
| C68 | 0.0473 (14) | 0.0402 (16) | 0.0406 (15) | −0.0107 (12) | −0.0151 (12) | −0.0003 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C6 | 1.407 (3) | C24—H24 | 0.9300 |
| O1—C7 | 1.372 (3) | C25—H25 | 0.9300 |
| O2—C7 | 1.184 (4) | C30—H30 | 0.9300 |
| O3—C14 | 1.223 (3) | C31—H31 | 0.9300 |
| O4—C27 | 1.212 (3) | C32—H32 | 0.9300 |
| O5—C28 | 1.217 (3) | C33—H33 | 0.9300 |
| O6—C40 | 1.405 (3) | C35—C36 | 1.387 (4) |
| O6—C41 | 1.364 (3) | C35—C40 | 1.382 (3) |
| O7—C41 | 1.200 (3) | C35—C50 | 1.491 (3) |

| | | | |
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| O8—C48 | 1.214 (3) | C36—C37 | 1.382 (4) |
| O9—C61 | 1.219 (3) | C37—C38 | 1.366 (4) |
| O10—C62 | 1.213 (3) | C38—C39 | 1.384 (4) |
| C1—C16 | 1.493 (3) | C39—C40 | 1.367 (4) |
| C1—C6 | 1.381 (4) | C41—C42 | 1.502 (4) |
| C1—C2 | 1.382 (4) | C42—C43 | 1.396 (3) |
| C2—C3 | 1.401 (5) | C42—C47 | 1.400 (3) |
| C3—C4 | 1.382 (5) | C43—C44 | 1.371 (4) |
| C4—C5 | 1.356 (5) | C44—C45 | 1.374 (4) |
| C5—C6 | 1.374 (4) | C45—C46 | 1.370 (4) |
| C7—C8 | 1.495 (4) | C46—C47 | 1.393 (3) |
| C8—C13 | 1.386 (4) | C47—C48 | 1.489 (3) |
| C8—C9 | 1.386 (4) | C48—C49 | 1.507 (3) |
| C9—C10 | 1.366 (5) | C49—C50 | 1.413 (3) |
| C10—C11 | 1.363 (5) | C49—C54 | 1.396 (3) |
| C11—C12 | 1.375 (4) | C50—C51 | 1.378 (3) |
| C12—C13 | 1.396 (4) | C51—C52 | 1.411 (3) |
| C13—C14 | 1.480 (4) | C51—C62 | 1.505 (4) |
| C14—C15 | 1.509 (3) | C52—C53 | 1.385 (3) |
| C15—C20 | 1.392 (3) | C52—C68 | 1.484 (3) |
| C15—C16 | 1.415 (3) | C53—C54 | 1.414 (3) |
| C16—C17 | 1.385 (3) | C53—C61 | 1.500 (3) |
| C17—C28 | 1.496 (3) | C54—C55 | 1.485 (3) |
| C17—C18 | 1.412 (3) | C55—C56 | 1.390 (3) |
| C18—C19 | 1.384 (3) | C55—C60 | 1.391 (3) |
| C18—C34 | 1.491 (3) | C56—C57 | 1.391 (4) |
| C19—C27 | 1.499 (3) | C57—C58 | 1.364 (4) |
| C19—C20 | 1.417 (3) | C58—C59 | 1.381 (4) |
| C20—C21 | 1.493 (3) | C59—C60 | 1.381 (4) |
| C21—C22 | 1.391 (4) | C60—C61 | 1.486 (4) |
| C21—C26 | 1.387 (3) | C62—C63 | 1.486 (4) |
| C22—C23 | 1.393 (4) | C63—C64 | 1.379 (4) |
| C23—C24 | 1.365 (4) | C63—C68 | 1.391 (3) |
| C24—C25 | 1.384 (4) | C64—C65 | 1.376 (4) |
| C25—C26 | 1.379 (4) | C65—C66 | 1.381 (4) |
| C26—C27 | 1.487 (4) | C66—C67 | 1.386 (4) |
| C28—C29 | 1.481 (4) | C67—C68 | 1.376 (4) |
| C29—C30 | 1.377 (4) | C36—H36 | 0.9300 |
| C29—C34 | 1.397 (3) | C37—H37 | 0.9300 |
| C30—C31 | 1.371 (4) | C38—H38 | 0.9300 |
| C31—C32 | 1.380 (4) | C39—H39 | 0.9300 |
| C32—C33 | 1.397 (4) | C43—H43 | 0.9300 |
| C33—C34 | 1.384 (3) | C44—H44 | 0.9300 |
| C2—H2 | 0.9300 | C45—H45 | 0.9300 |
| C3—H3 | 0.9300 | C46—H46 | 0.9300 |
| C4—H4 | 0.9300 | C56—H56 | 0.9300 |
| C5—H5 | 0.9300 | C57—H57 | 0.9300 |
| C9—H9 | 0.9300 | C58—H58 | 0.9300 |

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|---|---|---|---|
| C10—H10 | 0.9300 | C59—H59 | 0.9300 |
| C11—H11 | 0.9300 | C64—H64 | 0.9300 |
| C12—H12 | 0.9300 | C65—H65 | 0.9300 |
| C22—H22 | 0.9300 | C66—H66 | 0.9300 |
| C23—H23 | 0.9300 | C67—H67 | 0.9300 |
| | | | |
| C6—O1—C7 | 119.8 (2) | C34—C33—H33 | 121.00 |
| C40—O6—C41 | 118.32 (19) | C36—C35—C40 | 117.6 (2) |
| C2—C1—C6 | 117.7 (3) | C36—C35—C50 | 124.1 (2) |
| C6—C1—C16 | 118.7 (2) | C40—C35—C50 | 118.3 (2) |
| C2—C1—C16 | 123.5 (3) | C35—C36—C37 | 120.4 (2) |
| C1—C2—C3 | 119.9 (3) | C36—C37—C38 | 120.3 (3) |
| C2—C3—C4 | 119.5 (3) | C37—C38—C39 | 120.5 (2) |
| C3—C4—C5 | 121.5 (3) | C38—C39—C40 | 118.4 (2) |
| C4—C5—C6 | 117.9 (3) | O6—C40—C35 | 117.1 (2) |
| O1—C6—C1 | 116.9 (2) | O6—C40—C39 | 120.0 (2) |
| C1—C6—C5 | 123.5 (3) | C35—C40—C39 | 122.8 (2) |
| O1—C6—C5 | 119.4 (2) | O6—C41—O7 | 118.8 (2) |
| O1—C7—C8 | 115.4 (2) | O6—C41—C42 | 117.4 (2) |
| O2—C7—C8 | 126.7 (3) | O7—C41—C42 | 123.2 (2) |
| O1—C7—O2 | 117.5 (2) | C41—C42—C43 | 113.4 (2) |
| C7—C8—C9 | 114.1 (3) | C41—C42—C47 | 127.3 (2) |
| C9—C8—C13 | 119.6 (3) | C43—C42—C47 | 119.3 (2) |
| C7—C8—C13 | 126.2 (2) | C42—C43—C44 | 120.9 (2) |
| C8—C9—C10 | 120.6 (3) | C43—C44—C45 | 120.1 (2) |
| C9—C10—C11 | 120.3 (3) | C44—C45—C46 | 119.7 (2) |
| C10—C11—C12 | 120.4 (3) | C45—C46—C47 | 121.8 (2) |
| C11—C12—C13 | 120.3 (3) | C42—C47—C46 | 118.2 (2) |
| C8—C13—C12 | 118.9 (2) | C42—C47—C48 | 125.6 (2) |
| C12—C13—C14 | 115.6 (2) | C46—C47—C48 | 116.3 (2) |
| C8—C13—C14 | 125.5 (2) | O8—C48—C47 | 120.1 (2) |
| O3—C14—C13 | 119.3 (2) | O8—C48—C49 | 118.8 (2) |
| C13—C14—C15 | 124.9 (2) | C47—C48—C49 | 121.1 (2) |
| O3—C14—C15 | 115.8 (2) | C48—C49—C50 | 119.7 (2) |
| C14—C15—C20 | 119.5 (2) | C48—C49—C54 | 121.1 (2) |
| C16—C15—C20 | 119.0 (2) | C50—C49—C54 | 119.2 (2) |
| C14—C15—C16 | 120.9 (2) | C35—C50—C49 | 118.5 (2) |
| C1—C16—C17 | 120.0 (2) | C35—C50—C51 | 122.5 (2) |
| C15—C16—C17 | 118.8 (2) | C49—C50—C51 | 118.9 (2) |
| C1—C16—C15 | 121.1 (2) | C50—C51—C52 | 122.8 (2) |
| C16—C17—C28 | 129.3 (2) | C50—C51—C62 | 129.1 (2) |
| C18—C17—C28 | 108.1 (2) | C52—C51—C62 | 108.1 (2) |
| C16—C17—C18 | 122.7 (2) | C51—C52—C53 | 118.1 (2) |
| C17—C18—C19 | 118.3 (2) | C51—C52—C68 | 108.5 (2) |
| C19—C18—C34 | 133.3 (2) | C53—C52—C68 | 133.4 (2) |
| C17—C18—C34 | 108.4 (2) | C52—C53—C54 | 120.1 (2) |
| C18—C19—C20 | 119.8 (2) | C52—C53—C61 | 132.1 (2) |
| C20—C19—C27 | 108.3 (2) | C54—C53—C61 | 107.9 (2) |

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|---|---|---|---|
| C18—C19—C27 | 132.0 (2) | C49—C54—C53 | 120.8 (2) |
| C15—C20—C21 | 130.3 (2) | C49—C54—C55 | 130.5 (2) |
| C19—C20—C21 | 108.3 (2) | C53—C54—C55 | 108.6 (2) |
| C15—C20—C19 | 121.4 (2) | C54—C55—C56 | 132.4 (2) |
| C20—C21—C22 | 132.7 (2) | C54—C55—C60 | 108.3 (2) |
| C20—C21—C26 | 108.1 (2) | C56—C55—C60 | 119.3 (2) |
| C22—C21—C26 | 119.1 (2) | C55—C56—C57 | 118.1 (2) |
| C21—C22—C23 | 117.9 (2) | C56—C57—C58 | 121.9 (2) |
| C22—C23—C24 | 122.5 (3) | C57—C58—C59 | 120.8 (3) |
| C23—C24—C25 | 120.0 (2) | C58—C59—C60 | 117.9 (2) |
| C24—C25—C26 | 118.1 (2) | C55—C60—C59 | 122.1 (2) |
| C21—C26—C25 | 122.5 (2) | C55—C60—C61 | 109.5 (2) |
| C21—C26—C27 | 110.1 (2) | C59—C60—C61 | 128.4 (2) |
| C25—C26—C27 | 127.4 (2) | O9—C61—C53 | 128.1 (2) |
| O4—C27—C19 | 128.0 (2) | O9—C61—C60 | 126.4 (2) |
| O4—C27—C26 | 126.9 (2) | C53—C61—C60 | 105.4 (2) |
| C19—C27—C26 | 105.1 (2) | O10—C62—C51 | 127.0 (2) |
| O5—C28—C29 | 126.9 (2) | O10—C62—C63 | 127.8 (2) |
| C17—C28—C29 | 105.9 (2) | C51—C62—C63 | 105.2 (2) |
| O5—C28—C17 | 127.2 (2) | C62—C63—C64 | 128.8 (2) |
| C28—C29—C30 | 128.9 (2) | C62—C63—C68 | 109.6 (2) |
| C30—C29—C34 | 121.8 (2) | C64—C63—C68 | 121.6 (2) |
| C28—C29—C34 | 109.3 (2) | C63—C64—C65 | 118.5 (2) |
| C29—C30—C31 | 118.2 (2) | C64—C65—C66 | 120.0 (3) |
| C30—C31—C32 | 121.0 (2) | C65—C66—C67 | 121.7 (3) |
| C31—C32—C33 | 121.3 (2) | C66—C67—C68 | 118.3 (2) |
| C32—C33—C34 | 117.9 (2) | C52—C68—C63 | 108.6 (2) |
| C18—C34—C29 | 108.3 (2) | C52—C68—C67 | 131.6 (2) |
| C29—C34—C33 | 119.8 (2) | C63—C68—C67 | 119.8 (2) |
| C18—C34—C33 | 131.8 (2) | C35—C36—H36 | 120.00 |
| C1—C2—H2 | 120.00 | C37—C36—H36 | 120.00 |
| C3—C2—H2 | 120.00 | C36—C37—H37 | 120.00 |
| C4—C3—H3 | 120.00 | C38—C37—H37 | 120.00 |
| C2—C3—H3 | 120.00 | C37—C38—H38 | 120.00 |
| C5—C4—H4 | 119.00 | C39—C38—H38 | 120.00 |
| C3—C4—H4 | 119.00 | C38—C39—H39 | 121.00 |
| C4—C5—H5 | 121.00 | C40—C39—H39 | 121.00 |
| C6—C5—H5 | 121.00 | C42—C43—H43 | 120.00 |
| C8—C9—H9 | 120.00 | C44—C43—H43 | 120.00 |
| C10—C9—H9 | 120.00 | C43—C44—H44 | 120.00 |
| C11—C10—H10 | 120.00 | C45—C44—H44 | 120.00 |
| C9—C10—H10 | 120.00 | C44—C45—H45 | 120.00 |
| C10—C11—H11 | 120.00 | C46—C45—H45 | 120.00 |
| C12—C11—H11 | 120.00 | C45—C46—H46 | 119.00 |
| C13—C12—H12 | 120.00 | C47—C46—H46 | 119.00 |
| C11—C12—H12 | 120.00 | C55—C56—H56 | 121.00 |
| C21—C22—H22 | 121.00 | C57—C56—H56 | 121.00 |
| C23—C22—H22 | 121.00 | C56—C57—H57 | 119.00 |

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|---|---|---|---|
| C24—C23—H23 | 119.00 | C58—C57—H57 | 119.00 |
| C22—C23—H23 | 119.00 | C57—C58—H58 | 120.00 |
| C23—C24—H24 | 120.00 | C59—C58—H58 | 120.00 |
| C25—C24—H24 | 120.00 | C58—C59—H59 | 121.00 |
| C26—C25—H25 | 121.00 | C60—C59—H59 | 121.00 |
| C24—C25—H25 | 121.00 | C63—C64—H64 | 121.00 |
| C29—C30—H30 | 121.00 | C65—C64—H64 | 121.00 |
| C31—C30—H30 | 121.00 | C64—C65—H65 | 120.00 |
| C32—C31—H31 | 119.00 | C66—C65—H65 | 120.00 |
| C30—C31—H31 | 119.00 | C65—C66—H66 | 119.00 |
| C31—C32—H32 | 119.00 | C67—C66—H66 | 119.00 |
| C33—C32—H32 | 119.00 | C66—C67—H67 | 121.00 |
| C32—C33—H33 | 121.00 | C68—C67—H67 | 121.00 |
| | | | |
| C7—O1—C6—C1 | −76.7 (3) | C30—C31—C32—C33 | 0.2 (4) |
| C7—O1—C6—C5 | 107.8 (3) | C31—C32—C33—C34 | 0.2 (4) |
| C6—O1—C7—O2 | 166.9 (2) | C32—C33—C34—C18 | −179.5 (2) |
| C6—O1—C7—C8 | −20.1 (3) | C32—C33—C34—C29 | −0.5 (4) |
| C40—O6—C41—C42 | 32.3 (3) | C50—C35—C40—O6 | −5.5 (3) |
| C41—O6—C40—C35 | 69.9 (3) | C50—C35—C40—C39 | 178.5 (2) |
| C41—O6—C40—C39 | −114.0 (3) | C36—C35—C50—C49 | 90.7 (3) |
| C40—O6—C41—O7 | −156.0 (2) | C36—C35—C50—C51 | −93.5 (3) |
| C16—C1—C6—C5 | 175.9 (2) | C40—C35—C50—C49 | −87.4 (3) |
| C2—C1—C16—C15 | −102.7 (3) | C40—C35—C50—C51 | 88.4 (3) |
| C2—C1—C16—C17 | 79.1 (3) | C36—C35—C40—O6 | 176.3 (2) |
| C16—C1—C6—O1 | 0.5 (3) | C36—C35—C40—C39 | 0.3 (4) |
| C16—C1—C2—C3 | −175.6 (2) | C40—C35—C36—C37 | −0.8 (4) |
| C2—C1—C6—O1 | −175.7 (2) | C50—C35—C36—C37 | −178.9 (2) |
| C2—C1—C6—C5 | −0.3 (4) | C35—C36—C37—C38 | 0.9 (4) |
| C6—C1—C16—C15 | 81.4 (3) | C36—C37—C38—C39 | −0.4 (4) |
| C6—C1—C16—C17 | −96.8 (3) | C37—C38—C39—C40 | −0.1 (4) |
| C6—C1—C2—C3 | 0.3 (4) | C38—C39—C40—O6 | −175.8 (2) |
| C1—C2—C3—C4 | −0.4 (4) | C38—C39—C40—C35 | 0.1 (4) |
| C2—C3—C4—C5 | 0.4 (5) | O6—C41—C42—C43 | 93.9 (3) |
| C3—C4—C5—C6 | −0.4 (5) | O6—C41—C42—C47 | −88.4 (3) |
| C4—C5—C6—C1 | 0.3 (4) | O7—C41—C42—C43 | −77.4 (3) |
| C4—C5—C6—O1 | 175.6 (3) | O7—C41—C42—C47 | 100.3 (3) |
| O2—C7—C8—C13 | −98.7 (4) | C41—C42—C43—C44 | 176.9 (2) |
| O1—C7—C8—C9 | −92.2 (3) | C47—C42—C43—C44 | −1.0 (4) |
| O1—C7—C8—C13 | 89.0 (3) | C41—C42—C47—C46 | −177.4 (2) |
| O2—C7—C8—C9 | 80.1 (3) | C41—C42—C47—C48 | 1.4 (4) |
| C13—C8—C9—C10 | −0.4 (4) | C43—C42—C47—C46 | 0.2 (3) |
| C7—C8—C13—C12 | 177.7 (2) | C43—C42—C47—C48 | 179.0 (2) |
| C7—C8—C9—C10 | −179.3 (3) | C42—C43—C44—C45 | 0.9 (4) |
| C7—C8—C13—C14 | −1.3 (4) | C43—C44—C45—C46 | 0.0 (4) |
| C9—C8—C13—C12 | −1.1 (4) | C44—C45—C46—C47 | −0.9 (4) |
| C9—C8—C13—C14 | 179.9 (2) | C45—C46—C47—C42 | 0.7 (4) |
| C8—C9—C10—C11 | 1.5 (5) | C45—C46—C47—C48 | −178.2 (2) |

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|---|---|---|---|
| C9—C10—C11—C12 | −1.3 (5) | C42—C47—C48—O8 | 172.3 (2) |
| C10—C11—C12—C13 | −0.2 (5) | C42—C47—C48—C49 | −9.8 (4) |
| C11—C12—C13—C8 | 1.4 (4) | C46—C47—C48—O8 | −8.8 (4) |
| C11—C12—C13—C14 | −179.5 (3) | C46—C47—C48—C49 | 169.1 (2) |
| C12—C13—C14—C15 | 173.4 (2) | O8—C48—C49—C50 | −104.7 (3) |
| C12—C13—C14—O3 | −7.1 (4) | O8—C48—C49—C54 | 74.2 (3) |
| C8—C13—C14—O3 | 172.0 (2) | C47—C48—C49—C50 | 77.4 (3) |
| C8—C13—C14—C15 | −7.5 (4) | C47—C48—C49—C54 | −103.8 (3) |
| O3—C14—C15—C20 | −57.0 (3) | C48—C49—C50—C35 | −4.8 (3) |
| C13—C14—C15—C16 | −66.4 (3) | C48—C49—C50—C51 | 179.3 (2) |
| C13—C14—C15—C20 | 122.5 (3) | C54—C49—C50—C35 | 176.3 (2) |
| O3—C14—C15—C16 | 114.1 (3) | C54—C49—C50—C51 | 0.4 (3) |
| C14—C15—C20—C19 | 169.2 (2) | C48—C49—C54—C53 | 177.8 (2) |
| C14—C15—C20—C21 | −12.7 (4) | C48—C49—C54—C55 | −0.7 (4) |
| C16—C15—C20—C19 | −2.1 (3) | C50—C49—C54—C53 | −3.3 (3) |
| C14—C15—C16—C1 | 12.4 (3) | C50—C49—C54—C55 | 178.1 (2) |
| C14—C15—C16—C17 | −169.4 (2) | C35—C50—C51—C52 | −174.9 (2) |
| C20—C15—C16—C1 | −176.5 (2) | C35—C50—C51—C62 | 3.5 (4) |
| C20—C15—C16—C17 | 1.8 (3) | C49—C50—C51—C52 | 0.9 (4) |
| C16—C15—C20—C21 | 176.0 (2) | C49—C50—C51—C62 | 179.3 (2) |
| C15—C16—C17—C28 | −177.8 (2) | C50—C51—C52—C53 | 0.7 (3) |
| C1—C16—C17—C18 | 178.6 (2) | C50—C51—C52—C68 | −178.8 (2) |
| C1—C16—C17—C28 | 0.4 (4) | C62—C51—C52—C53 | −177.9 (2) |
| C15—C16—C17—C18 | 0.4 (4) | C62—C51—C52—C68 | 2.5 (3) |
| C16—C17—C18—C34 | 178.5 (2) | C50—C51—C62—O10 | 0.0 (4) |
| C28—C17—C18—C19 | 176.3 (2) | C50—C51—C62—C63 | 179.6 (2) |
| C16—C17—C18—C19 | −2.3 (4) | C52—C51—C62—O10 | 178.5 (3) |
| C18—C17—C28—C29 | 3.2 (3) | C52—C51—C62—C63 | −1.8 (3) |
| C16—C17—C28—O5 | 3.2 (4) | C51—C52—C53—C54 | −3.6 (3) |
| C16—C17—C28—C29 | −178.4 (2) | C51—C52—C53—C61 | 176.0 (2) |
| C28—C17—C18—C34 | −3.0 (3) | C68—C52—C53—C54 | 175.8 (2) |
| C18—C17—C28—O5 | −175.2 (3) | C68—C52—C53—C61 | −4.6 (5) |
| C17—C18—C19—C20 | 1.9 (3) | C51—C52—C68—C63 | −2.3 (3) |
| C17—C18—C19—C27 | −177.0 (2) | C51—C52—C68—C67 | 176.5 (3) |
| C19—C18—C34—C29 | −177.5 (3) | C53—C52—C68—C63 | 178.3 (3) |
| C19—C18—C34—C33 | 1.7 (5) | C53—C52—C68—C67 | −3.0 (5) |
| C17—C18—C34—C33 | −179.3 (3) | C52—C53—C54—C49 | 5.0 (3) |
| C34—C18—C19—C20 | −179.1 (2) | C52—C53—C54—C55 | −176.2 (2) |
| C34—C18—C19—C27 | 2.1 (5) | C61—C53—C54—C49 | −174.7 (2) |
| C17—C18—C34—C29 | 1.6 (3) | C61—C53—C54—C55 | 4.2 (3) |
| C18—C19—C20—C21 | −178.3 (2) | C52—C53—C61—O9 | −8.4 (4) |
| C27—C19—C20—C15 | 179.3 (2) | C52—C53—C61—C60 | 175.4 (2) |
| C27—C19—C20—C21 | 0.9 (3) | C54—C53—C61—O9 | 171.2 (2) |
| C18—C19—C20—C15 | 0.2 (4) | C54—C53—C61—C60 | −5.1 (3) |
| C18—C19—C27—O4 | −3.8 (5) | C49—C54—C55—C56 | −3.9 (4) |
| C18—C19—C27—C26 | 176.9 (2) | C49—C54—C55—C60 | 177.1 (2) |
| C20—C19—C27—O4 | 177.3 (3) | C53—C54—C55—C56 | 177.5 (3) |
| C20—C19—C27—C26 | −2.1 (3) | C53—C54—C55—C60 | −1.6 (3) |

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| C15—C20—C21—C26 | −177.5 (2) | C54—C55—C56—C57 | −178.9 (2) |
| C19—C20—C21—C22 | 178.0 (3) | C60—C55—C56—C57 | 0.1 (4) |
| C15—C20—C21—C22 | −0.3 (5) | C54—C55—C60—C59 | 179.4 (2) |
| C19—C20—C21—C26 | 0.8 (3) | C54—C55—C60—C61 | −1.7 (3) |
| C20—C21—C26—C27 | −2.2 (3) | C56—C55—C60—C59 | 0.2 (4) |
| C22—C21—C26—C27 | −179.8 (2) | C56—C55—C60—C61 | 179.1 (2) |
| C26—C21—C22—C23 | 0.8 (4) | C55—C56—C57—C58 | 0.6 (4) |
| C22—C21—C26—C25 | −0.4 (4) | C56—C57—C58—C59 | −1.6 (4) |
| C20—C21—C22—C23 | −176.2 (3) | C57—C58—C59—C60 | 1.8 (4) |
| C20—C21—C26—C25 | 177.3 (2) | C58—C59—C60—C55 | −1.1 (4) |
| C21—C22—C23—C24 | −0.4 (4) | C58—C59—C60—C61 | −179.8 (2) |
| C22—C23—C24—C25 | −0.4 (4) | C55—C60—C61—O9 | −172.2 (2) |
| C23—C24—C25—C26 | 0.8 (4) | C55—C60—C61—C53 | 4.1 (3) |
| C24—C25—C26—C21 | −0.4 (4) | C59—C60—C61—O9 | 6.7 (4) |
| C24—C25—C26—C27 | 179.0 (2) | C59—C60—C61—C53 | −177.0 (2) |
| C21—C26—C27—C19 | 2.6 (3) | O10—C62—C63—C64 | 2.3 (5) |
| C25—C26—C27—O4 | 3.9 (4) | O10—C62—C63—C68 | −179.9 (3) |
| C21—C26—C27—O4 | −176.7 (3) | C51—C62—C63—C64 | −177.4 (2) |
| C25—C26—C27—C19 | −176.8 (2) | C51—C62—C63—C68 | 0.4 (3) |
| C17—C28—C29—C34 | −2.2 (3) | C62—C63—C64—C65 | 177.1 (3) |
| C17—C28—C29—C30 | 178.5 (2) | C68—C63—C64—C65 | −0.5 (4) |
| O5—C28—C29—C30 | −3.1 (4) | C62—C63—C68—C52 | 1.1 (3) |
| O5—C28—C29—C34 | 176.2 (3) | C62—C63—C68—C67 | −177.9 (2) |
| C34—C29—C30—C31 | −0.3 (4) | C64—C63—C68—C52 | 179.1 (2) |
| C28—C29—C34—C18 | 0.4 (3) | C64—C63—C68—C67 | 0.2 (4) |
| C28—C29—C34—C33 | −178.8 (2) | C63—C64—C65—C66 | 0.4 (4) |
| C28—C29—C30—C31 | 179.0 (3) | C64—C65—C66—C67 | 0.1 (4) |
| C30—C29—C34—C18 | 179.8 (2) | C65—C66—C67—C68 | −0.5 (4) |
| C30—C29—C34—C33 | 0.6 (4) | C66—C67—C68—C52 | −178.3 (3) |
| C29—C30—C31—C32 | −0.1 (4) | C66—C67—C68—C63 | 0.3 (4) |

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| C12—H12···O3 | 0.93 | 2.37 | 2.693 (3) | 100 |
| C22—H22···O3 | 0.93 | 2.50 | 3.081 (3) | 121 |
| C24—H24···O10[i] | 0.93 | 2.56 | 3.302 (3) | 137 |
| C30—H30···O5[ii] | 0.93 | 2.60 | 3.507 (3) | 166 |
| C32—H32···O7[iii] | 0.93 | 2.49 | 3.398 (3) | 166 |
| C33—H33···O4 | 0.93 | 2.32 | 3.087 (3) | 139 |
| C39—H39···O1[iv] | 0.93 | 2.36 | 3.115 (3) | 139 |
| C46—H46···O8 | 0.93 | 2.40 | 2.728 (3) | 101 |
| C56—H56···O8 | 0.93 | 2.52 | 3.210 (3) | 131 |
| C58—H58···O7[v] | 0.93 | 2.52 | 3.377 (3) | 154 |
| C67—H67···O9 | 0.93 | 2.36 | 3.117 (3) | 139 |

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