Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (2*RS*,3*SR*,10*SR*,11*RS*)-3,10-Diphenoxy-18,21-dioxa-5,8-diazapentacyclo-[20.4.0.0$^{2,5}$.0$^{8,11}$.0$^{12,17}$]hexacosa-1(26),12,14,16,22,24-hexaene-4,9-dione ethyl acetate hemisolvate

**J. Suresh,[a] Natarajan Arumugam,[b] Abdulrahman I. Almansour,[b] Usama Karama[b] and P. L. Nilantha Lakshman[c]***

[a]Department of Physics, The Madura College, Madurai 625 011, India, [b]Department of Chemistry, College of Sciences, King Saud University, PO Box 2455, Riyadh 11451, Saudi Arabia, and [c]Department of Food Science and Technology, University of Ruhuna, Mapalana, Kamburupitiya 81100, Sri Lanka
Correspondence e-mail: plakshmannilantha@ymail.com

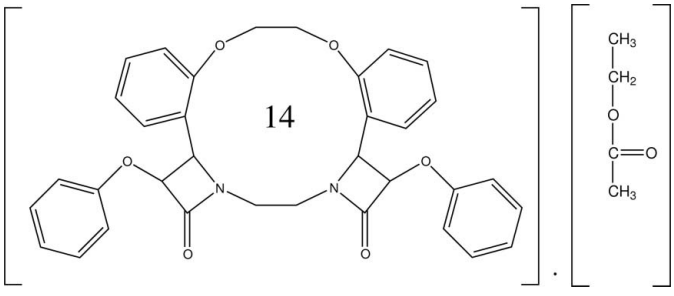
Received 22 July 2011; accepted 26 July 2011

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.053; $wR$ factor = 0.175; data-to-parameter ratio = 16.2.

In the title compound, $C_{34}H_{30}N_2O_6\cdot0.5C_4H_8O_2$, there are two molecules in the asymmetric unit and the structure is stabilized by C—H···O interactions. The two nonsolvent molecules of the asymmetric unit are linked together by a weak C—H···O hydrogen bond. The ethyl acetate molecule is present as a space filler and does not participate in the hydrogen-bonding network.

## Related literature

For background to the pharmaceutical applications of $\beta$-lactam antibiotics, see: Samarendra *et al.* (1994); Vaccaro & Davis (1998); Vaccaro *et al.* (1998); Borthwick *et al.* (1998).




## Experimental

### Crystal data

$C_{34}H_{30}N_2O_6\cdot0.5(C_4H_8O_2)$
$M_r$ = 606.65
Monoclinic, $P2_1/n$
$a$ = 18.037 (3) Å
$b$ = 17.201 (3) Å
$c$ = 21.589 (4) Å
$\beta$ = 108.722 (1)°
$V$ = 6343.67 (19) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 K
0.18 × 0.16 × 0.13 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min}$ = 0.984, $T_{max}$ = 0.988
64493 measured reflections
13208 independent reflections
7192 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.046

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.175
$S$ = 1.02
13208 reflections
813 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C53—H53···O6 | 0.93 | 2.52 | 3.344 (3) | 147 |
| C2—H2···O2 | 0.93 | 2.42 | 3.250 (3) | 149 |
| C32—H32···O1 | 0.93 | 2.33 | 3.178 (3) | 151 |
| C66—H66···O7 | 0.93 | 2.48 | 3.299 (3) | 147 |

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

NA, AIA and UK extend their appreciation to the Deanship of Scientific Research at King Saud University for their funding of this work through the research grant No. RGP-VPP-026.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2069).

## References

Borthwick, A. D., Weingarte, G., Haley, T. M., Tomaszewski, M., Wang, W., Hu, Z., Bedard, J., Jin, H., Yuen, L. & Mansour, T. S. (1998). *Bioorg. Med. Chem. Lett.* **8**, 365–370.
Bruker (1998). *SADABS*. Bruker AXS Inc., Maddison, Wisconsin, USA.
Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Samarendra, C. I., Maiti, N., Micetich, R., Daneshtalab, M., Atchison, K., Phillips, O. A. & Kunugita, C. (1994). *J. Antibiot.* **47**, 1030–1040.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Vaccaro, W. D. & Davis, H. R. Jr (1998). *Bioorg. Med. Chem. Lett.* **8**, 313–318.
Vaccaro, W. D., Sher, R. & Davis, H. R. Jr (1998). *Bioorg. Med. Chem. Lett.* **8**, 35–40.

# supporting information

*Acta Cryst.* (2011). E**67**, o2203 [doi:10.1107/S1600536811030200]

# (2*RS*,3*SR*,10*SR*,11*RS*)-3,10-Diphenoxy-18,21-dioxa-5,8-diazapentacyclo-[20.4.0.0$^{2,5}$.0$^{8,11}$.0$^{12,17}$]hexacosa-1(26),12,14,16,22,24-hexaene-4,9-dione ethyl acetate hemisolvate

**J. Suresh, Natarajan Arumugam, Abdulrahman I. Almansour, Usama Karama and P. L. Nilantha Lakshman**

## S1. Comment

*β*-Lactam antibiotics are widely employed in the treatment of bacterial infections(Samarendra *et al.*, 1994). In recent years, several natural *β*-lactams have been shown to exhibit a high antibacterial activity. 1,3,4-trisubstituted *β*-lactams were found to be new, potent cholesterol absorption inhibitors (Vaccaro & Davis 1998; Vaccaro *et al.*, 1998) human cytomegalovirus (Borthwick *et al.*, 1998). Furthermore, many anticancer drugs in current use are toxic and thus limited in their efficacy. It is therefore essential to develop novel chemotherapeutic agents with lower levels of toxicity. *β*-lactam antibiotics have been used for many years with limited or no toxicity. In view of this, the crystal structure determination of the title compound was carried out.

The asymmetric unit of (I) contain two independent molecules, The pair have almost identical geometry. The internal angles of the four-membered rings of the title compound, (I), vary from 85.3 (8) to 96.2 (5)° . The sums of the bond angles at the N atoms are 359.4 (2) and 360.0 (1),359.3 (8) 359.9 (5) for N1, N2,N3 and N4 respectively are in accordance with $sp^2$ hybridization. The conformation of the molecules is stabilized by weak intramolecular C—H···O and C—H···N interactions, (Table 1). The two non-solvent molecules of the asymmetruc unit are linked together by a weak C—H···O hydrogen bond. The presence of the ethyl acetate solvent as a mere space filler suggests that its contribution to the intermolecular interactions is insignificant but it has nevertheless played a role in crystallization. There is a solvent accessible void of 66.7 Å$^3$ in the structure.

## S2. Experimental

A solution of phenoxyacetyl chloride in dry dichloromethane (20 ml) was slowly added to a solution of bisimine (1 mmol) and $Et_3N$ (3.5 mmol) in dichloromethane (20 ml) at 0 °C and the reaction mixture was stirred for 12 h at room temperature. Completion of the reaction evidenced by TLC analysis, the reaction mixture was washed with water (2 *X* 20 ml), saturated $NaHCO_3$ (15 ml) and brine (15 ml). The organic layer was dried over anhydrous $Na_2SO_4$ and concentrated under reduced pressure. The crude product was separated by column chromatography (hexane: ethyl acetate 7:3) gave pure bis-*β*-lactam in good yield. The product was recrystallized from ethyl acetate by slow evaporation technique. m.p.: 195°C, yield: 48%

## S3. Refinement

The H atoms were placed in calculated positions and allowed to ride on their carrier atoms with C—H = 0.93–0.98 Å and $U_{iso}$ = 1.2$U_{eq}$(C,) for CH, $CH_2$ groups and $U_{iso}$ = 1.5$U_{eq}$(C) for $CH_3$ group.

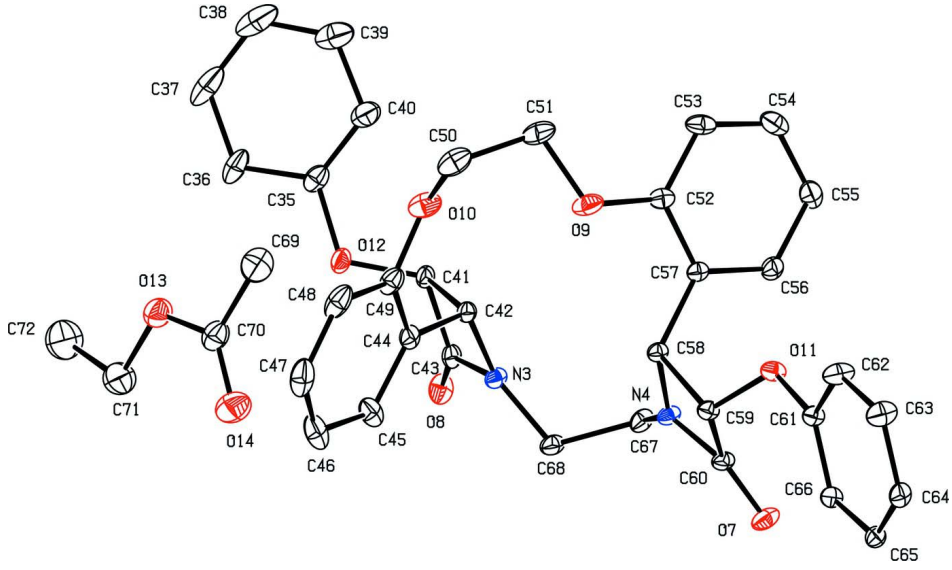



**Figure 1**

One of the molecule of the two independent molecules and the solvent molecule ethyl acetate of the asymmetric unit(I), showing 10% probability displacement ellipsoids and the atom-numbering scheme. H-atoms are omitted for clarity.

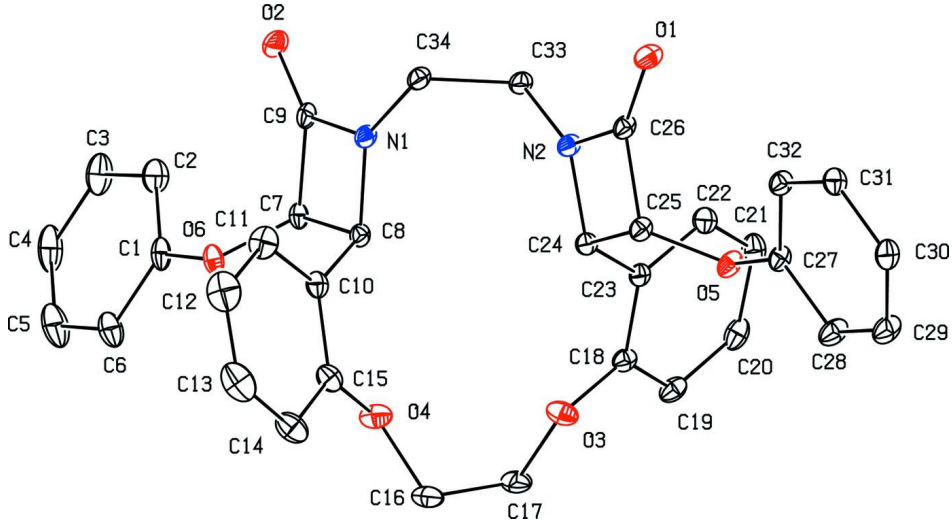



**Figure 2**

The other molecule of the two independent molecules of the asymmetric unit(I), showing 10% probability displacement ellipsoids and the atom-numbering scheme. H-atoms are omitted for clarity.

## (2*RS*,3*SR*,10*SR*,11*RS*)-3,10-Diphenoxy-18,21-dioxa-5,8- diazapentacyclo[20.4.0.0$^{2,5}$.0$^{8,11}$.0$^{12,17}$]hexacosa-1(26),12,14,16,22,24-hexaene-4,9-dione ethyl acetate hemisolvate

*Crystal data*

$C_{34}H_{30}N_2O_6{\cdot}0.5(C_4H_8O_2)$
$M_r$ = 606.65
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 18.037 (3) Å
$b$ = 17.201 (3) Å
$c$ = 21.589 (4) Å
$\beta$ = 108.722 (10)°
$V$ = 6343.67 (19) Å$^3$
$Z$ = 8

$F(000) = 2560$
$D_x = 1.270$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 2500 reflections
$\theta = 2–27°$
$\mu = 0.09$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.18 × 0.16 × 0.13 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.984$, $T_{max} = 0.988$
64493 measured reflections
13208 independent reflections
7192 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 26.6°$, $\theta_{min} = 1.7°$
$h = -22\rightarrow22$
$k = -21\rightarrow21$
$l = -27\rightarrow27$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.175$
$S = 1.02$
13208 reflections
813 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
$w = 1/[\sigma^2(F_o^2) + (0.0801P)^2 + 1.3813P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å$^{-3}$
$\Delta\rho_{min} = -0.24$ e Å$^{-3}$

*Special details*

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

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

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.58820 (10) | 0.50849 (11) | 0.49402 (8) | 0.0675 (5) |
| O2 | 0.46252 (10) | 0.40807 (11) | 0.76094 (9) | 0.0678 (5) |
| O3 | 0.79089 (11) | 0.27095 (10) | 0.67869 (9) | 0.0692 (5) |
| O4 | 0.68980 (10) | 0.18393 (11) | 0.72407 (9) | 0.0723 (5) |
| O5 | 0.75451 (8) | 0.41331 (10) | 0.52020 (7) | 0.0543 (4) |
| O6 | 0.54253 (9) | 0.23356 (9) | 0.79798 (7) | 0.0546 (4) |
| N1 | 0.53463 (10) | 0.36778 (11) | 0.69396 (9) | 0.0482 (5) |
| N2 | 0.62448 (10) | 0.43556 (11) | 0.59046 (8) | 0.0477 (5) |
| C1 | 0.53443 (14) | 0.23039 (16) | 0.85949 (11) | 0.0579 (7) |
| C2 | 0.50667 (17) | 0.29204 (19) | 0.88634 (13) | 0.0738 (8) |
| H2 | 0.4938 | 0.3387 | 0.8636 | 0.089* |
| C3 | 0.49799 (19) | 0.2840 (2) | 0.94753 (15) | 0.0934 (11) |

| | | | | |
|---|---|---|---|---|
| H3 | 0.4790 | 0.3253 | 0.9658 | 0.112* |
| C4 | 0.5172 (2) | 0.2159 (3) | 0.98101 (16) | 0.1071 (14) |
| H4 | 0.5124 | 0.2110 | 1.0225 | 0.129* |
| C5 | 0.5436 (2) | 0.1545 (3) | 0.95333 (17) | 0.1107 (13) |
| H5 | 0.5555 | 0.1078 | 0.9760 | 0.133* |
| C6 | 0.55309 (18) | 0.16067 (19) | 0.89231 (14) | 0.0805 (9) |
| H6 | 0.5715 | 0.1190 | 0.8740 | 0.097* |
| C7 | 0.56993 (12) | 0.30462 (13) | 0.78045 (10) | 0.0451 (5) |
| H7 | 0.6143 | 0.3252 | 0.8160 | 0.054* |
| C8 | 0.58797 (12) | 0.30110 (13) | 0.71428 (10) | 0.0438 (5) |
| H8 | 0.6423 | 0.3153 | 0.7197 | 0.053* |
| C9 | 0.51115 (12) | 0.36898 (14) | 0.74746 (11) | 0.0481 (6) |
| C10 | 0.56317 (14) | 0.22914 (14) | 0.67387 (10) | 0.0501 (6) |
| C11 | 0.48777 (17) | 0.2166 (2) | 0.63373 (13) | 0.0766 (8) |
| H11 | 0.4499 | 0.2545 | 0.6302 | 0.092* |
| C12 | 0.4673 (2) | 0.1484 (3) | 0.59849 (16) | 0.1033 (12) |
| H12 | 0.4158 | 0.1405 | 0.5721 | 0.124* |
| C13 | 0.5221 (3) | 0.0930 (2) | 0.60227 (17) | 0.1031 (12) |
| H13 | 0.5079 | 0.0477 | 0.5778 | 0.124* |
| C14 | 0.5990 (2) | 0.10279 (18) | 0.64218 (15) | 0.0818 (9) |
| H14 | 0.6365 | 0.0649 | 0.6444 | 0.098* |
| C15 | 0.61848 (16) | 0.17077 (15) | 0.67866 (12) | 0.0593 (6) |
| C16 | 0.75889 (17) | 0.15158 (17) | 0.71566 (17) | 0.0795 (9) |
| H16A | 0.7482 | 0.1332 | 0.6712 | 0.095* |
| H16B | 0.7776 | 0.1082 | 0.7453 | 0.095* |
| C17 | 0.81814 (16) | 0.21491 (17) | 0.73031 (15) | 0.0751 (8) |
| H17A | 0.8231 | 0.2385 | 0.7722 | 0.090* |
| H17B | 0.8688 | 0.1946 | 0.7317 | 0.090* |
| C18 | 0.81363 (13) | 0.34669 (15) | 0.69163 (10) | 0.0488 (6) |
| C19 | 0.88309 (14) | 0.36788 (17) | 0.73889 (11) | 0.0582 (7) |
| H19 | 0.9157 | 0.3301 | 0.7645 | 0.070* |
| C20 | 0.90333 (15) | 0.4447 (2) | 0.74750 (13) | 0.0669 (8) |
| H20 | 0.9498 | 0.4589 | 0.7793 | 0.080* |
| C21 | 0.85609 (17) | 0.50128 (18) | 0.70996 (13) | 0.0675 (7) |
| H21 | 0.8704 | 0.5534 | 0.7161 | 0.081* |
| C22 | 0.78640 (15) | 0.47960 (15) | 0.66253 (11) | 0.0559 (6) |
| H22 | 0.7543 | 0.5177 | 0.6370 | 0.067* |
| C23 | 0.76414 (12) | 0.40245 (13) | 0.65274 (10) | 0.0426 (5) |
| C24 | 0.68875 (12) | 0.37855 (13) | 0.60175 (10) | 0.0439 (5) |
| H24 | 0.6725 | 0.3259 | 0.6090 | 0.053* |
| C25 | 0.68248 (12) | 0.39336 (14) | 0.52855 (10) | 0.0466 (5) |
| H25 | 0.6570 | 0.3500 | 0.5002 | 0.056* |
| C26 | 0.62359 (12) | 0.45784 (15) | 0.53028 (10) | 0.0482 (6) |
| C27 | 0.75411 (12) | 0.42248 (14) | 0.45610 (10) | 0.0476 (5) |
| C28 | 0.81786 (15) | 0.39355 (18) | 0.44128 (12) | 0.0685 (8) |
| H28 | 0.8577 | 0.3679 | 0.4730 | 0.082* |
| C29 | 0.82196 (16) | 0.40302 (18) | 0.37899 (13) | 0.0721 (8) |
| H29 | 0.8649 | 0.3837 | 0.3690 | 0.087* |

| | | | | |
|---|---|---|---|---|
| C30 | 0.76339 (15) | 0.44063 (16) | 0.33156 (12) | 0.0611 (7) |
| H30 | 0.7662 | 0.4462 | 0.2895 | 0.073* |
| C31 | 0.70102 (14) | 0.46967 (15) | 0.34697 (11) | 0.0546 (6) |
| H31 | 0.6615 | 0.4957 | 0.3152 | 0.066* |
| C32 | 0.69594 (13) | 0.46082 (14) | 0.40911 (11) | 0.0507 (6) |
| H32 | 0.6532 | 0.4808 | 0.4190 | 0.061* |
| C33 | 0.58264 (13) | 0.46822 (14) | 0.63199 (11) | 0.0504 (6) |
| H33A | 0.5624 | 0.5188 | 0.6149 | 0.061* |
| H33B | 0.6195 | 0.4760 | 0.6755 | 0.061* |
| C34 | 0.51501 (12) | 0.41862 (15) | 0.63752 (11) | 0.0526 (6) |
| H34A | 0.4729 | 0.4528 | 0.6391 | 0.063* |
| H34B | 0.4956 | 0.3871 | 0.5983 | 0.063* |
| O7 | 0.08612 (10) | −0.03084 (12) | 0.50260 (9) | 0.0732 (6) |
| O8 | −0.02514 (11) | 0.08467 (11) | 0.77821 (10) | 0.0750 (5) |
| O9 | 0.27029 (12) | 0.22602 (11) | 0.67684 (9) | 0.0814 (6) |
| O10 | 0.18251 (14) | 0.31822 (12) | 0.73090 (10) | 0.0873 (6) |
| O11 | 0.23893 (8) | 0.08131 (10) | 0.51517 (7) | 0.0545 (4) |
| O12 | 0.05351 (10) | 0.25116 (10) | 0.81692 (8) | 0.0634 (5) |
| N3 | 0.03988 (10) | 0.12389 (12) | 0.70535 (9) | 0.0516 (5) |
| N4 | 0.11730 (10) | 0.05203 (11) | 0.59366 (8) | 0.0495 (5) |
| C35 | 0.10712 (19) | 0.29037 (16) | 0.86937 (13) | 0.0687 (7) |
| C36 | 0.0732 (3) | 0.33826 (19) | 0.90397 (16) | 0.1016 (12) |
| H36 | 0.0191 | 0.3433 | 0.8925 | 0.122* |
| C37 | 0.1232 (4) | 0.3788 (3) | 0.9568 (2) | 0.146 (2) |
| H37 | 0.1017 | 0.4126 | 0.9801 | 0.176* |
| C38 | 0.2030 (4) | 0.3706 (3) | 0.9758 (3) | 0.158 (2) |
| H38 | 0.2352 | 0.3967 | 1.0123 | 0.190* |
| C39 | 0.2332 (3) | 0.3238 (3) | 0.9400 (2) | 0.1273 (15) |
| H39 | 0.2873 | 0.3184 | 0.9520 | 0.153* |
| C40 | 0.1864 (2) | 0.2834 (2) | 0.88599 (16) | 0.0918 (10) |
| H40 | 0.2087 | 0.2522 | 0.8616 | 0.110* |
| C41 | 0.08090 (14) | 0.18611 (14) | 0.79130 (11) | 0.0506 (6) |
| H41 | 0.1279 | 0.1642 | 0.8232 | 0.061* |
| C42 | 0.09050 (13) | 0.19243 (13) | 0.72190 (11) | 0.0471 (5) |
| H42 | 0.1441 | 0.1811 | 0.7228 | 0.057* |
| C43 | 0.02096 (14) | 0.12327 (14) | 0.76097 (11) | 0.0521 (6) |
| C44 | 0.05858 (15) | 0.26504 (16) | 0.68418 (11) | 0.0562 (6) |
| C45 | −0.01947 (17) | 0.2737 (2) | 0.64774 (13) | 0.0765 (9) |
| H45 | −0.0540 | 0.2326 | 0.6448 | 0.092* |
| C46 | −0.0471 (2) | 0.3434 (3) | 0.61535 (15) | 0.1036 (14) |
| H46 | −0.1000 | 0.3491 | 0.5921 | 0.124* |
| C47 | 0.0032 (3) | 0.4026 (3) | 0.61783 (17) | 0.1100 (15) |
| H47 | −0.0149 | 0.4479 | 0.5944 | 0.132* |
| C48 | 0.0809 (3) | 0.39636 (19) | 0.65468 (16) | 0.1004 (12) |
| H48 | 0.1149 | 0.4377 | 0.6571 | 0.120* |
| C49 | 0.1083 (2) | 0.32766 (17) | 0.68836 (13) | 0.0713 (8) |
| C50 | 0.2471 (2) | 0.34862 (19) | 0.71346 (19) | 0.0998 (11) |
| H50A | 0.2698 | 0.3930 | 0.7406 | 0.120* |

| | | | | |
|---|---|---|---|---|
| H50B | 0.2299 | 0.3650 | 0.6681 | 0.120* |
| C51 | 0.3058 (2) | 0.2846 (2) | 0.72398 (17) | 0.0935 (10) |
| H51A | 0.3535 | 0.3034 | 0.7177 | 0.112* |
| H51B | 0.3184 | 0.2640 | 0.7680 | 0.112* |
| C52 | 0.30210 (13) | 0.15310 (15) | 0.68510 (11) | 0.0536 (6) |
| C53 | 0.37626 (15) | 0.1362 (2) | 0.72771 (13) | 0.0705 (8) |
| H53 | 0.4073 | 0.1757 | 0.7522 | 0.085* |
| C54 | 0.40356 (16) | 0.0618 (2) | 0.73372 (14) | 0.0803 (9) |
| H54 | 0.4531 | 0.0508 | 0.7625 | 0.096* |
| C55 | 0.35892 (18) | 0.0031 (2) | 0.69790 (13) | 0.0774 (9) |
| H55 | 0.3780 | −0.0476 | 0.7020 | 0.093* |
| C56 | 0.28482 (15) | 0.01966 (16) | 0.65534 (11) | 0.0592 (6) |
| H56 | 0.2542 | −0.0204 | 0.6313 | 0.071* |
| C57 | 0.25554 (12) | 0.09451 (13) | 0.64801 (10) | 0.0427 (5) |
| C58 | 0.17667 (12) | 0.11307 (13) | 0.59957 (10) | 0.0436 (5) |
| H58 | 0.1580 | 0.1652 | 0.6055 | 0.052* |
| C59 | 0.16737 (12) | 0.09423 (14) | 0.52655 (10) | 0.0474 (5) |
| H59 | 0.1360 | 0.1338 | 0.4969 | 0.057* |
| C60 | 0.11648 (13) | 0.02564 (16) | 0.53458 (11) | 0.0522 (6) |
| C61 | 0.23611 (12) | 0.07508 (14) | 0.45046 (10) | 0.0461 (5) |
| C62 | 0.29714 (16) | 0.10742 (19) | 0.43439 (13) | 0.0752 (9) |
| H62 | 0.3367 | 0.1339 | 0.4658 | 0.090* |
| C63 | 0.29951 (17) | 0.10048 (19) | 0.37165 (13) | 0.0788 (9) |
| H63 | 0.3409 | 0.1225 | 0.3609 | 0.095* |
| C64 | 0.24212 (15) | 0.06174 (15) | 0.32478 (11) | 0.0571 (6) |
| H64 | 0.2443 | 0.0574 | 0.2825 | 0.069* |
| C65 | 0.18145 (14) | 0.02940 (14) | 0.34073 (11) | 0.0516 (6) |
| H65 | 0.1422 | 0.0028 | 0.3092 | 0.062* |
| C66 | 0.17816 (13) | 0.03615 (14) | 0.40402 (10) | 0.0489 (6) |
| H66 | 0.1367 | 0.0143 | 0.4147 | 0.059* |
| C67 | 0.08087 (14) | 0.02224 (15) | 0.63947 (12) | 0.0567 (6) |
| H67A | 0.1210 | 0.0153 | 0.6815 | 0.068* |
| H67B | 0.0591 | −0.0286 | 0.6246 | 0.068* |
| C68 | 0.01636 (13) | 0.07316 (17) | 0.64897 (12) | 0.0628 (7) |
| H68A | −0.0050 | 0.1049 | 0.6101 | 0.075* |
| H68B | −0.0253 | 0.0397 | 0.6526 | 0.075* |
| O13 | 0.64589 (13) | 0.69087 (14) | 0.51650 (12) | 0.1002 (7) |
| O14 | 0.67151 (18) | 0.64668 (18) | 0.61737 (13) | 0.1269 (9) |
| C69 | 0.5398 (2) | 0.6845 (2) | 0.5557 (2) | 0.1183 (13) |
| H69A | 0.5112 | 0.6431 | 0.5285 | 0.178* |
| H69B | 0.5238 | 0.7333 | 0.5340 | 0.178* |
| H69C | 0.5293 | 0.6843 | 0.5965 | 0.178* |
| C70 | 0.6249 (2) | 0.6732 (2) | 0.56792 (18) | 0.0894 (10) |
| C71 | 0.7275 (2) | 0.6741 (3) | 0.5224 (2) | 0.1394 (17) |
| H71A | 0.7626 | 0.7059 | 0.5564 | 0.167* |
| H71B | 0.7394 | 0.6198 | 0.5333 | 0.167* |
| C72 | 0.7356 (3) | 0.6917 (4) | 0.4603 (3) | 0.187 (3) |
| H72A | 0.6979 | 0.6625 | 0.4268 | 0.280* |

| | | | | |
|---|---|---|---|---|
| H72B | 0.7874 | 0.6782 | 0.4607 | 0.280* |
| H72C | 0.7270 | 0.7463 | 0.4515 | 0.280* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0629 (10) | 0.0937 (14) | 0.0532 (10) | 0.0301 (10) | 0.0288 (8) | 0.0327 (10) |
| O2 | 0.0679 (11) | 0.0809 (13) | 0.0716 (12) | 0.0114 (10) | 0.0459 (10) | 0.0080 (10) |
| O3 | 0.0805 (12) | 0.0558 (12) | 0.0588 (11) | 0.0143 (10) | 0.0050 (9) | 0.0102 (9) |
| O4 | 0.0673 (11) | 0.0669 (12) | 0.0752 (13) | 0.0155 (9) | 0.0121 (10) | −0.0115 (10) |
| O5 | 0.0451 (8) | 0.0895 (12) | 0.0327 (8) | 0.0076 (8) | 0.0188 (7) | 0.0068 (8) |
| O6 | 0.0673 (10) | 0.0610 (10) | 0.0375 (8) | −0.0207 (8) | 0.0196 (7) | 0.0042 (7) |
| N1 | 0.0469 (10) | 0.0603 (12) | 0.0444 (11) | 0.0092 (9) | 0.0243 (8) | 0.0148 (9) |
| N2 | 0.0472 (10) | 0.0637 (12) | 0.0382 (10) | 0.0142 (9) | 0.0219 (8) | 0.0149 (9) |
| C1 | 0.0575 (14) | 0.0792 (19) | 0.0360 (13) | −0.0279 (13) | 0.0135 (11) | 0.0048 (13) |
| C2 | 0.0846 (19) | 0.093 (2) | 0.0494 (16) | −0.0148 (17) | 0.0288 (14) | 0.0006 (15) |
| C3 | 0.103 (2) | 0.133 (3) | 0.0557 (19) | −0.039 (2) | 0.0420 (17) | −0.010 (2) |
| C4 | 0.121 (3) | 0.161 (4) | 0.0485 (19) | −0.064 (3) | 0.0388 (19) | 0.002 (2) |
| C5 | 0.145 (3) | 0.122 (3) | 0.065 (2) | −0.044 (3) | 0.033 (2) | 0.030 (2) |
| C6 | 0.099 (2) | 0.083 (2) | 0.0595 (18) | −0.0216 (18) | 0.0262 (16) | 0.0180 (16) |
| C7 | 0.0476 (12) | 0.0528 (14) | 0.0373 (12) | −0.0109 (11) | 0.0171 (9) | 0.0042 (10) |
| C8 | 0.0429 (11) | 0.0527 (14) | 0.0388 (12) | 0.0010 (10) | 0.0173 (9) | 0.0097 (10) |
| C9 | 0.0450 (12) | 0.0607 (15) | 0.0455 (13) | −0.0054 (11) | 0.0242 (10) | 0.0057 (11) |
| C10 | 0.0571 (14) | 0.0587 (15) | 0.0357 (12) | −0.0058 (12) | 0.0168 (10) | 0.0061 (11) |
| C11 | 0.0685 (17) | 0.097 (2) | 0.0555 (17) | −0.0120 (16) | 0.0076 (14) | −0.0075 (16) |
| C12 | 0.102 (3) | 0.122 (3) | 0.065 (2) | −0.032 (3) | −0.0015 (18) | −0.015 (2) |
| C13 | 0.146 (4) | 0.083 (3) | 0.068 (2) | −0.034 (3) | 0.016 (2) | −0.0200 (19) |
| C14 | 0.118 (3) | 0.0595 (19) | 0.0642 (19) | −0.0030 (18) | 0.0242 (18) | −0.0039 (15) |
| C15 | 0.0758 (17) | 0.0550 (16) | 0.0455 (14) | −0.0040 (14) | 0.0169 (13) | 0.0033 (12) |
| C16 | 0.083 (2) | 0.0571 (18) | 0.100 (2) | 0.0284 (16) | 0.0317 (17) | 0.0122 (16) |
| C17 | 0.0671 (17) | 0.0720 (19) | 0.081 (2) | 0.0288 (16) | 0.0170 (15) | 0.0269 (16) |
| C18 | 0.0508 (13) | 0.0615 (16) | 0.0386 (12) | 0.0093 (12) | 0.0209 (10) | 0.0029 (11) |
| C19 | 0.0480 (13) | 0.085 (2) | 0.0441 (14) | 0.0124 (13) | 0.0180 (11) | 0.0007 (13) |
| C20 | 0.0535 (15) | 0.104 (2) | 0.0479 (15) | −0.0090 (16) | 0.0226 (12) | −0.0068 (15) |
| C21 | 0.0807 (19) | 0.0758 (19) | 0.0549 (16) | −0.0181 (16) | 0.0343 (15) | −0.0066 (15) |
| C22 | 0.0660 (15) | 0.0625 (17) | 0.0456 (14) | 0.0029 (13) | 0.0268 (12) | 0.0063 (12) |
| C23 | 0.0492 (12) | 0.0527 (14) | 0.0335 (11) | 0.0052 (11) | 0.0237 (10) | 0.0066 (10) |
| C24 | 0.0487 (12) | 0.0501 (13) | 0.0368 (12) | 0.0055 (10) | 0.0193 (10) | 0.0067 (10) |
| C25 | 0.0458 (12) | 0.0620 (15) | 0.0340 (11) | 0.0037 (11) | 0.0157 (9) | 0.0049 (10) |
| C26 | 0.0426 (12) | 0.0682 (16) | 0.0375 (12) | 0.0073 (11) | 0.0182 (10) | 0.0117 (11) |
| C27 | 0.0485 (12) | 0.0650 (15) | 0.0334 (12) | −0.0013 (11) | 0.0191 (10) | 0.0009 (11) |
| C28 | 0.0596 (15) | 0.105 (2) | 0.0479 (15) | 0.0214 (15) | 0.0276 (12) | 0.0132 (14) |
| C29 | 0.0701 (17) | 0.102 (2) | 0.0581 (17) | 0.0154 (16) | 0.0402 (14) | 0.0052 (15) |
| C30 | 0.0754 (17) | 0.0769 (18) | 0.0411 (14) | −0.0081 (14) | 0.0327 (13) | 0.0011 (13) |
| C31 | 0.0622 (15) | 0.0638 (16) | 0.0398 (13) | −0.0039 (12) | 0.0193 (11) | 0.0055 (11) |
| C32 | 0.0508 (13) | 0.0649 (16) | 0.0410 (13) | 0.0046 (12) | 0.0211 (10) | 0.0044 (11) |
| C33 | 0.0545 (13) | 0.0589 (15) | 0.0471 (13) | 0.0135 (11) | 0.0293 (11) | 0.0126 (11) |
| C34 | 0.0445 (12) | 0.0699 (16) | 0.0481 (13) | 0.0143 (11) | 0.0216 (10) | 0.0211 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O7 | 0.0749 (12) | 0.0944 (14) | 0.0594 (11) | −0.0356 (11) | 0.0341 (9) | −0.0355 (10) |
| O8 | 0.0878 (13) | 0.0758 (13) | 0.0845 (14) | −0.0058 (11) | 0.0600 (11) | −0.0011 (10) |
| O9 | 0.0924 (14) | 0.0577 (13) | 0.0716 (13) | −0.0242 (11) | −0.0050 (10) | −0.0041 (10) |
| O10 | 0.1087 (16) | 0.0700 (13) | 0.0707 (14) | −0.0264 (12) | 0.0113 (12) | 0.0074 (11) |
| O11 | 0.0440 (8) | 0.0917 (13) | 0.0311 (8) | −0.0079 (8) | 0.0167 (6) | −0.0012 (8) |
| O12 | 0.0800 (11) | 0.0635 (11) | 0.0474 (10) | 0.0159 (9) | 0.0216 (9) | −0.0108 (8) |
| N3 | 0.0498 (11) | 0.0667 (13) | 0.0455 (11) | −0.0117 (10) | 0.0253 (9) | −0.0141 (9) |
| N4 | 0.0491 (10) | 0.0665 (13) | 0.0386 (10) | −0.0179 (9) | 0.0223 (8) | −0.0150 (9) |
| C35 | 0.103 (2) | 0.0580 (17) | 0.0463 (15) | −0.0021 (16) | 0.0264 (15) | 0.0010 (13) |
| C36 | 0.167 (3) | 0.077 (2) | 0.073 (2) | 0.003 (2) | 0.057 (2) | −0.0237 (18) |
| C37 | 0.249 (6) | 0.098 (3) | 0.100 (4) | −0.018 (4) | 0.066 (4) | −0.048 (3) |
| C38 | 0.229 (7) | 0.122 (4) | 0.094 (4) | −0.050 (5) | 0.012 (4) | −0.036 (3) |
| C39 | 0.138 (4) | 0.112 (3) | 0.104 (3) | −0.036 (3) | 0.000 (3) | −0.011 (3) |
| C40 | 0.104 (3) | 0.084 (2) | 0.075 (2) | −0.008 (2) | 0.0113 (19) | −0.0140 (18) |
| C41 | 0.0604 (14) | 0.0524 (14) | 0.0397 (13) | 0.0122 (11) | 0.0171 (11) | −0.0046 (11) |
| C42 | 0.0459 (12) | 0.0529 (14) | 0.0460 (13) | 0.0001 (11) | 0.0196 (10) | −0.0070 (11) |
| C43 | 0.0567 (14) | 0.0582 (15) | 0.0508 (14) | 0.0069 (12) | 0.0304 (11) | −0.0009 (11) |
| C44 | 0.0662 (16) | 0.0708 (18) | 0.0381 (13) | 0.0129 (14) | 0.0256 (11) | −0.0018 (12) |
| C45 | 0.0727 (18) | 0.117 (3) | 0.0509 (16) | 0.0300 (18) | 0.0350 (14) | 0.0157 (16) |
| C46 | 0.113 (3) | 0.161 (4) | 0.0489 (18) | 0.076 (3) | 0.0432 (19) | 0.030 (2) |
| C47 | 0.184 (5) | 0.101 (3) | 0.053 (2) | 0.066 (3) | 0.048 (3) | 0.018 (2) |
| C48 | 0.183 (4) | 0.055 (2) | 0.058 (2) | 0.014 (2) | 0.032 (2) | 0.0022 (16) |
| C49 | 0.107 (2) | 0.0581 (18) | 0.0475 (16) | 0.0031 (17) | 0.0233 (16) | −0.0022 (13) |
| C50 | 0.130 (3) | 0.061 (2) | 0.105 (3) | −0.048 (2) | 0.034 (2) | −0.0126 (19) |
| C51 | 0.097 (2) | 0.073 (2) | 0.097 (3) | −0.045 (2) | 0.0135 (19) | −0.0191 (19) |
| C52 | 0.0526 (14) | 0.0641 (17) | 0.0454 (14) | −0.0168 (12) | 0.0172 (11) | 0.0019 (12) |
| C53 | 0.0490 (15) | 0.107 (3) | 0.0533 (16) | −0.0250 (16) | 0.0127 (12) | −0.0007 (16) |
| C54 | 0.0500 (16) | 0.137 (3) | 0.0536 (17) | 0.0135 (19) | 0.0158 (13) | 0.0057 (19) |
| C55 | 0.084 (2) | 0.101 (2) | 0.0478 (16) | 0.0341 (19) | 0.0209 (15) | 0.0052 (16) |
| C56 | 0.0702 (16) | 0.0669 (18) | 0.0413 (13) | 0.0053 (13) | 0.0189 (12) | −0.0057 (12) |
| C57 | 0.0461 (12) | 0.0563 (15) | 0.0304 (11) | −0.0085 (11) | 0.0188 (9) | −0.0011 (10) |
| C58 | 0.0445 (12) | 0.0527 (14) | 0.0359 (11) | −0.0063 (10) | 0.0163 (9) | −0.0038 (10) |
| C59 | 0.0430 (12) | 0.0665 (16) | 0.0340 (12) | −0.0027 (11) | 0.0143 (9) | −0.0018 (11) |
| C60 | 0.0435 (12) | 0.0775 (18) | 0.0381 (12) | −0.0106 (12) | 0.0167 (10) | −0.0148 (12) |
| C61 | 0.0471 (12) | 0.0612 (15) | 0.0330 (11) | −0.0030 (11) | 0.0169 (10) | 0.0027 (10) |
| C62 | 0.0686 (17) | 0.114 (2) | 0.0489 (15) | −0.0386 (17) | 0.0273 (13) | −0.0134 (15) |
| C63 | 0.0793 (19) | 0.116 (3) | 0.0559 (17) | −0.0335 (18) | 0.0419 (15) | −0.0120 (16) |
| C64 | 0.0710 (16) | 0.0698 (17) | 0.0387 (13) | 0.0068 (13) | 0.0291 (12) | 0.0011 (12) |
| C65 | 0.0555 (13) | 0.0596 (15) | 0.0407 (13) | 0.0043 (12) | 0.0171 (10) | −0.0047 (11) |
| C66 | 0.0466 (12) | 0.0619 (15) | 0.0415 (13) | −0.0039 (11) | 0.0188 (10) | 0.0009 (11) |
| C67 | 0.0663 (15) | 0.0621 (16) | 0.0539 (14) | −0.0193 (12) | 0.0365 (12) | −0.0153 (12) |
| C68 | 0.0493 (13) | 0.091 (2) | 0.0537 (15) | −0.0201 (13) | 0.0249 (11) | −0.0268 (14) |
| O13 | 0.0974 (16) | 0.1138 (19) | 0.0950 (17) | 0.0069 (14) | 0.0389 (13) | 0.0220 (14) |
| O14 | 0.144 (2) | 0.143 (3) | 0.0833 (18) | 0.0065 (19) | 0.0226 (17) | 0.0098 (17) |
| C69 | 0.123 (3) | 0.116 (3) | 0.137 (4) | 0.025 (3) | 0.071 (3) | 0.013 (3) |
| C70 | 0.117 (3) | 0.080 (2) | 0.073 (2) | −0.003 (2) | 0.032 (2) | 0.0031 (18) |
| C71 | 0.096 (3) | 0.187 (5) | 0.148 (4) | 0.013 (3) | 0.056 (3) | 0.046 (4) |
| C72 | 0.139 (4) | 0.261 (7) | 0.190 (6) | 0.011 (4) | 0.094 (4) | 0.060 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C26 | 1.208 (3) | O11—C59 | 1.407 (2) |
| O2—C9 | 1.213 (3) | O12—C35 | 1.403 (3) |
| O3—C18 | 1.368 (3) | O12—C41 | 1.406 (3) |
| O3—C17 | 1.436 (3) | N3—C43 | 1.350 (3) |
| O4—C15 | 1.363 (3) | N3—C68 | 1.446 (3) |
| O4—C16 | 1.428 (3) | N3—C42 | 1.463 (3) |
| O5—C27 | 1.390 (2) | N4—C60 | 1.349 (3) |
| O5—C25 | 1.410 (2) | N4—C67 | 1.446 (3) |
| O6—C1 | 1.383 (3) | N4—C58 | 1.476 (3) |
| O6—C7 | 1.415 (2) | C35—C40 | 1.364 (4) |
| N1—C9 | 1.352 (3) | C35—C36 | 1.380 (4) |
| N1—C34 | 1.448 (3) | C36—C37 | 1.394 (6) |
| N1—C8 | 1.471 (3) | C36—H36 | 0.9300 |
| N2—C26 | 1.350 (3) | C37—C38 | 1.370 (7) |
| N2—C33 | 1.457 (3) | C37—H37 | 0.9300 |
| N2—C24 | 1.478 (3) | C38—C39 | 1.346 (7) |
| C1—C2 | 1.377 (4) | C38—H38 | 0.9300 |
| C1—C6 | 1.379 (4) | C39—C40 | 1.387 (5) |
| C2—C3 | 1.386 (4) | C39—H39 | 0.9300 |
| C2—H2 | 0.9300 | C40—H40 | 0.9300 |
| C3—C4 | 1.362 (5) | C41—C43 | 1.520 (3) |
| C3—H3 | 0.9300 | C41—C42 | 1.566 (3) |
| C4—C5 | 1.373 (5) | C41—H41 | 0.9800 |
| C4—H4 | 0.9300 | C42—C44 | 1.501 (3) |
| C5—C6 | 1.386 (4) | C42—H42 | 0.9800 |
| C5—H5 | 0.9300 | C44—C45 | 1.383 (4) |
| C6—H6 | 0.9300 | C44—C49 | 1.385 (4) |
| C7—C9 | 1.540 (3) | C45—C46 | 1.397 (5) |
| C7—C8 | 1.565 (3) | C45—H45 | 0.9300 |
| C7—H7 | 0.9800 | C46—C47 | 1.355 (6) |
| C8—C10 | 1.498 (3) | C46—H46 | 0.9300 |
| C8—H8 | 0.9800 | C47—C48 | 1.375 (6) |
| C10—C11 | 1.375 (3) | C47—H47 | 0.9300 |
| C10—C15 | 1.396 (3) | C48—C49 | 1.392 (4) |
| C11—C12 | 1.382 (5) | C48—H48 | 0.9300 |
| C11—H11 | 0.9300 | C50—C51 | 1.493 (5) |
| C12—C13 | 1.355 (5) | C50—H50A | 0.9700 |
| C12—H12 | 0.9300 | C50—H50B | 0.9700 |
| C13—C14 | 1.389 (5) | C51—H51A | 0.9700 |
| C13—H13 | 0.9300 | C51—H51B | 0.9700 |
| C14—C15 | 1.390 (4) | C52—C53 | 1.389 (4) |
| C14—H14 | 0.9300 | C52—C57 | 1.389 (3) |
| C16—C17 | 1.487 (4) | C53—C54 | 1.363 (4) |
| C16—H16A | 0.9700 | C53—H53 | 0.9300 |
| C16—H16B | 0.9700 | C54—C55 | 1.366 (4) |
| C17—H17A | 0.9700 | C54—H54 | 0.9300 |

| | | | |
|---|---|---|---|
| C17—H17B | 0.9700 | C55—C56 | 1.387 (4) |
| C18—C19 | 1.387 (3) | C55—H55 | 0.9300 |
| C18—C23 | 1.393 (3) | C56—C57 | 1.381 (3) |
| C19—C20 | 1.368 (4) | C56—H56 | 0.9300 |
| C19—H19 | 0.9300 | C57—C58 | 1.505 (3) |
| C20—C21 | 1.373 (4) | C58—C59 | 1.565 (3) |
| C20—H20 | 0.9300 | C58—H58 | 0.9800 |
| C21—C22 | 1.393 (4) | C59—C60 | 1.538 (3) |
| C21—H21 | 0.9300 | C59—H59 | 0.9800 |
| C22—C23 | 1.383 (3) | C61—C66 | 1.369 (3) |
| C22—H22 | 0.9300 | C61—C62 | 1.374 (3) |
| C23—C24 | 1.506 (3) | C62—C63 | 1.374 (3) |
| C24—C25 | 1.569 (3) | C62—H62 | 0.9300 |
| C24—H24 | 0.9800 | C63—C64 | 1.366 (4) |
| C25—C26 | 1.544 (3) | C63—H63 | 0.9300 |
| C25—H25 | 0.9800 | C64—C65 | 1.367 (3) |
| C27—C32 | 1.372 (3) | C64—H64 | 0.9300 |
| C27—C28 | 1.382 (3) | C65—C66 | 1.391 (3) |
| C28—C29 | 1.380 (3) | C65—H65 | 0.9300 |
| C28—H28 | 0.9300 | C66—H66 | 0.9300 |
| C29—C30 | 1.374 (4) | C67—C68 | 1.522 (3) |
| C29—H29 | 0.9300 | C67—H67A | 0.9700 |
| C30—C31 | 1.366 (3) | C67—H67B | 0.9700 |
| C30—H30 | 0.9300 | C68—H68A | 0.9700 |
| C31—C32 | 1.382 (3) | C68—H68B | 0.9700 |
| C31—H31 | 0.9300 | O13—C70 | 1.319 (4) |
| C32—H32 | 0.9300 | O13—C71 | 1.464 (4) |
| C33—C34 | 1.524 (3) | O14—C70 | 1.216 (4) |
| C33—H33A | 0.9700 | C69—C70 | 1.484 (5) |
| C33—H33B | 0.9700 | C69—H69A | 0.9600 |
| C34—H34A | 0.9700 | C69—H69B | 0.9600 |
| C34—H34B | 0.9700 | C69—H69C | 0.9600 |
| O7—C60 | 1.216 (3) | C71—C72 | 1.428 (6) |
| O8—C43 | 1.212 (3) | C71—H71A | 0.9700 |
| O9—C52 | 1.367 (3) | C71—H71B | 0.9700 |
| O9—C51 | 1.429 (3) | C72—H72A | 0.9600 |
| O10—C49 | 1.369 (4) | C72—H72B | 0.9600 |
| O10—C50 | 1.434 (4) | C72—H72C | 0.9600 |
| O11—C61 | 1.386 (2) | | |

| | | | |
|---|---|---|---|
| C18—O3—C17 | 118.4 (2) | C40—C35—O12 | 124.3 (3) |
| C15—O4—C16 | 120.3 (2) | C36—C35—O12 | 114.4 (3) |
| C27—O5—C25 | 116.36 (16) | C35—C36—C37 | 117.3 (4) |
| C1—O6—C7 | 116.40 (18) | C35—C36—H36 | 121.3 |
| C9—N1—C34 | 130.60 (19) | C37—C36—H36 | 121.3 |
| C9—N1—C8 | 96.39 (16) | C38—C37—C36 | 122.3 (5) |
| C34—N1—C8 | 132.96 (17) | C38—C37—H37 | 118.8 |
| C26—N2—C33 | 129.37 (19) | C36—C37—H37 | 118.8 |

| | | | |
|---|---|---|---|
| C26—N2—C24 | 96.51 (16) | C39—C38—C37 | 118.0 (5) |
| C33—N2—C24 | 133.49 (17) | C39—C38—H38 | 121.0 |
| C2—C1—C6 | 121.0 (2) | C37—C38—H38 | 121.0 |
| C2—C1—O6 | 122.6 (2) | C38—C39—C40 | 122.2 (5) |
| C6—C1—O6 | 116.4 (3) | C38—C39—H39 | 118.9 |
| C1—C2—C3 | 119.5 (3) | C40—C39—H39 | 118.9 |
| C1—C2—H2 | 120.3 | C35—C40—C39 | 118.7 (4) |
| C3—C2—H2 | 120.3 | C35—C40—H40 | 120.6 |
| C4—C3—C2 | 120.3 (4) | C39—C40—H40 | 120.6 |
| C4—C3—H3 | 119.9 | O12—C41—C43 | 116.36 (19) |
| C2—C3—H3 | 119.9 | O12—C41—C42 | 118.80 (19) |
| C3—C4—C5 | 119.7 (3) | C43—C41—C42 | 85.36 (16) |
| C3—C4—H4 | 120.1 | O12—C41—H41 | 111.3 |
| C5—C4—H4 | 120.1 | C43—C41—H41 | 111.3 |
| C4—C5—C6 | 121.4 (4) | C42—C41—H41 | 111.3 |
| C4—C5—H5 | 119.3 | N3—C42—C44 | 115.9 (2) |
| C6—C5—H5 | 119.3 | N3—C42—C41 | 85.74 (16) |
| C1—C6—C5 | 118.1 (3) | C44—C42—C41 | 115.83 (18) |
| C1—C6—H6 | 121.0 | N3—C42—H42 | 112.3 |
| C5—C6—H6 | 121.0 | C44—C42—H42 | 112.3 |
| O6—C7—C9 | 119.80 (17) | C41—C42—H42 | 112.3 |
| O6—C7—C8 | 113.81 (18) | O8—C43—N3 | 132.2 (2) |
| C9—C7—C8 | 85.39 (15) | O8—C43—C41 | 136.1 (2) |
| O6—C7—H7 | 111.8 | N3—C43—C41 | 91.69 (17) |
| C9—C7—H7 | 111.8 | C45—C44—C49 | 118.2 (3) |
| C8—C7—H7 | 111.8 | C45—C44—C42 | 122.8 (3) |
| N1—C8—C10 | 115.24 (18) | C49—C44—C42 | 119.0 (2) |
| N1—C8—C7 | 86.23 (15) | C44—C45—C46 | 120.8 (3) |
| C10—C8—C7 | 116.93 (17) | C44—C45—H45 | 119.6 |
| N1—C8—H8 | 112.0 | C46—C45—H45 | 119.6 |
| C10—C8—H8 | 112.0 | C47—C46—C45 | 119.9 (4) |
| C7—C8—H8 | 112.0 | C47—C46—H46 | 120.0 |
| O2—C9—N1 | 131.5 (2) | C45—C46—H46 | 120.0 |
| O2—C9—C7 | 137.0 (2) | C46—C47—C48 | 120.6 (4) |
| N1—C9—C7 | 91.51 (17) | C46—C47—H47 | 119.7 |
| C11—C10—C15 | 118.2 (3) | C48—C47—H47 | 119.7 |
| C11—C10—C8 | 123.2 (2) | C47—C48—C49 | 119.5 (4) |
| C15—C10—C8 | 118.6 (2) | C47—C48—H48 | 120.2 |
| C10—C11—C12 | 121.1 (3) | C49—C48—H48 | 120.2 |
| C10—C11—H11 | 119.5 | O10—C49—C44 | 115.1 (2) |
| C12—C11—H11 | 119.5 | O10—C49—C48 | 123.9 (3) |
| C13—C12—C11 | 120.2 (3) | C44—C49—C48 | 120.8 (3) |
| C13—C12—H12 | 119.9 | O10—C50—C51 | 106.7 (3) |
| C11—C12—H12 | 119.9 | O10—C50—H50A | 110.4 |
| C12—C13—C14 | 121.1 (3) | C51—C50—H50A | 110.4 |
| C12—C13—H13 | 119.5 | O10—C50—H50B | 110.4 |
| C14—C13—H13 | 119.5 | C51—C50—H50B | 110.4 |
| C13—C14—C15 | 118.3 (3) | H50A—C50—H50B | 108.6 |

| | | | |
|---|---|---|---|
| C13—C14—H14 | 120.9 | O9—C51—C50 | 106.1 (3) |
| C15—C14—H14 | 120.9 | O9—C51—H51A | 110.5 |
| O4—C15—C14 | 123.7 (3) | C50—C51—H51A | 110.5 |
| O4—C15—C10 | 114.9 (2) | O9—C51—H51B | 110.5 |
| C14—C15—C10 | 121.2 (3) | C50—C51—H51B | 110.5 |
| O4—C16—C17 | 106.5 (2) | H51A—C51—H51B | 108.7 |
| O4—C16—H16A | 110.4 | O9—C52—C53 | 123.6 (2) |
| C17—C16—H16A | 110.4 | O9—C52—C57 | 116.1 (2) |
| O4—C16—H16B | 110.4 | C53—C52—C57 | 120.4 (3) |
| C17—C16—H16B | 110.4 | C54—C53—C52 | 120.1 (3) |
| H16A—C16—H16B | 108.6 | C54—C53—H53 | 120.0 |
| O3—C17—C16 | 106.4 (2) | C52—C53—H53 | 120.0 |
| O3—C17—H17A | 110.4 | C53—C54—C55 | 120.7 (3) |
| C16—C17—H17A | 110.4 | C53—C54—H54 | 119.6 |
| O3—C17—H17B | 110.4 | C55—C54—H54 | 119.6 |
| C16—C17—H17B | 110.4 | C54—C55—C56 | 119.4 (3) |
| H17A—C17—H17B | 108.6 | C54—C55—H55 | 120.3 |
| O3—C18—C19 | 122.8 (2) | C56—C55—H55 | 120.3 |
| O3—C18—C23 | 116.1 (2) | C57—C56—C55 | 121.3 (3) |
| C19—C18—C23 | 121.0 (2) | C57—C56—H56 | 119.3 |
| C20—C19—C18 | 119.5 (3) | C55—C56—H56 | 119.4 |
| C20—C19—H19 | 120.2 | C56—C57—C52 | 118.2 (2) |
| C18—C19—H19 | 120.2 | C56—C57—C58 | 121.3 (2) |
| C19—C20—C21 | 121.1 (3) | C52—C57—C58 | 120.6 (2) |
| C19—C20—H20 | 119.5 | N4—C58—C57 | 114.02 (18) |
| C21—C20—H20 | 119.5 | N4—C58—C59 | 85.72 (15) |
| C20—C21—C22 | 119.1 (3) | C57—C58—C59 | 115.33 (17) |
| C20—C21—H21 | 120.4 | N4—C58—H58 | 113.0 |
| C22—C21—H21 | 120.4 | C57—C58—H58 | 113.0 |
| C23—C22—C21 | 121.2 (2) | C59—C58—H58 | 113.0 |
| C23—C22—H22 | 119.4 | O11—C59—C60 | 120.8 (2) |
| C21—C22—H22 | 119.4 | O11—C59—C58 | 113.64 (17) |
| C22—C23—C18 | 118.0 (2) | C60—C59—C58 | 85.43 (15) |
| C22—C23—C24 | 121.6 (2) | O11—C59—H59 | 111.5 |
| C18—C23—C24 | 120.4 (2) | C60—C59—H59 | 111.5 |
| N2—C24—C23 | 114.57 (18) | C58—C59—H59 | 111.5 |
| N2—C24—C25 | 85.82 (15) | O7—C60—N4 | 132.2 (2) |
| C23—C24—C25 | 116.63 (17) | O7—C60—C59 | 136.5 (2) |
| N2—C24—H24 | 112.4 | N4—C60—C59 | 91.30 (18) |
| C23—C24—H24 | 112.4 | C66—C61—C62 | 119.9 (2) |
| C25—C24—H24 | 112.4 | C66—C61—O11 | 123.28 (18) |
| O5—C25—C26 | 119.82 (19) | C62—C61—O11 | 116.8 (2) |
| O5—C25—C24 | 113.38 (17) | C61—C62—C63 | 119.7 (2) |
| C26—C25—C24 | 85.41 (15) | C61—C62—H62 | 120.2 |
| O5—C25—H25 | 111.9 | C63—C62—H62 | 120.2 |
| C26—C25—H25 | 111.9 | C64—C63—C62 | 121.1 (2) |
| C24—C25—H25 | 111.9 | C64—C63—H63 | 119.4 |
| O1—C26—N2 | 132.0 (2) | C62—C63—H63 | 119.4 |

| | | | |
|---|---|---|---|
| O1—C26—C25 | 136.64 (19) | C63—C64—C65 | 119.3 (2) |
| N2—C26—C25 | 91.35 (17) | C63—C64—H64 | 120.3 |
| C32—C27—C28 | 119.9 (2) | C65—C64—H64 | 120.3 |
| C32—C27—O5 | 123.30 (19) | C64—C65—C66 | 120.2 (2) |
| C28—C27—O5 | 116.8 (2) | C64—C65—H65 | 119.9 |
| C29—C28—C27 | 119.5 (2) | C66—C65—H65 | 119.9 |
| C29—C28—H28 | 120.3 | C61—C66—C65 | 119.8 (2) |
| C27—C28—H28 | 120.3 | C61—C66—H66 | 120.1 |
| C30—C29—C28 | 120.9 (2) | C65—C66—H66 | 120.1 |
| C30—C29—H29 | 119.6 | N4—C67—C68 | 115.0 (2) |
| C28—C29—H29 | 119.6 | N4—C67—H67A | 108.5 |
| C31—C30—C29 | 119.1 (2) | C68—C67—H67A | 108.5 |
| C31—C30—H30 | 120.4 | N4—C67—H67B | 108.5 |
| C29—C30—H30 | 120.4 | C68—C67—H67B | 108.5 |
| C30—C31—C32 | 120.8 (2) | H67A—C67—H67B | 107.5 |
| C30—C31—H31 | 119.6 | N3—C68—C67 | 115.5 (2) |
| C32—C31—H31 | 119.6 | N3—C68—H68A | 108.4 |
| C27—C32—C31 | 119.8 (2) | C67—C68—H68A | 108.4 |
| C27—C32—H32 | 120.1 | N3—C68—H68B | 108.4 |
| C31—C32—H32 | 120.1 | C67—C68—H68B | 108.4 |
| N2—C33—C34 | 114.7 (2) | H68A—C68—H68B | 107.5 |
| N2—C33—H33A | 108.6 | C70—O13—C71 | 115.7 (3) |
| C34—C33—H33A | 108.6 | C70—C69—H69A | 109.5 |
| N2—C33—H33B | 108.6 | C70—C69—H69B | 109.5 |
| C34—C33—H33B | 108.6 | H69A—C69—H69B | 109.5 |
| H33A—C33—H33B | 107.6 | C70—C69—H69C | 109.5 |
| N1—C34—C33 | 114.73 (18) | H69A—C69—H69C | 109.5 |
| N1—C34—H34A | 108.6 | H69B—C69—H69C | 109.5 |
| C33—C34—H34A | 108.6 | O14—C70—O13 | 121.4 (4) |
| N1—C34—H34B | 108.6 | O14—C70—C69 | 126.2 (4) |
| C33—C34—H34B | 108.6 | O13—C70—C69 | 112.3 (3) |
| H34A—C34—H34B | 107.6 | C72—C71—O13 | 106.2 (4) |
| C52—O9—C51 | 118.7 (2) | C72—C71—H71A | 110.5 |
| C49—O10—C50 | 118.9 (2) | O13—C71—H71A | 110.5 |
| C61—O11—C59 | 116.70 (16) | C72—C71—H71B | 110.5 |
| C35—O12—C41 | 117.5 (2) | O13—C71—H71B | 110.5 |
| C43—N3—C68 | 130.9 (2) | H71A—C71—H71B | 108.7 |
| C43—N3—C42 | 96.04 (17) | C71—C72—H72A | 109.5 |
| C68—N3—C42 | 133.09 (18) | C71—C72—H72B | 109.5 |
| C60—N4—C67 | 131.1 (2) | H72A—C72—H72B | 109.5 |
| C60—N4—C58 | 96.23 (16) | C71—C72—H72C | 109.5 |
| C67—N4—C58 | 132.03 (17) | H72A—C72—H72C | 109.5 |
| C40—C35—C36 | 121.3 (3) | H72B—C72—H72C | 109.5 |
| | | | |
| C7—O6—C1—C2 | 39.0 (3) | C40—C35—C36—C37 | −0.4 (5) |
| C7—O6—C1—C6 | −143.2 (2) | O12—C35—C36—C37 | 179.8 (3) |
| C6—C1—C2—C3 | 0.5 (4) | C35—C36—C37—C38 | −1.9 (7) |
| O6—C1—C2—C3 | 178.2 (2) | C36—C37—C38—C39 | 2.6 (9) |

| | | | |
|---|---|---|---|
| C1—C2—C3—C4 | 0.4 (5) | C37—C38—C39—C40 | −1.0 (8) |
| C2—C3—C4—C5 | −1.4 (5) | C36—C35—C40—C39 | 1.9 (5) |
| C3—C4—C5—C6 | 1.5 (6) | O12—C35—C40—C39 | −178.4 (3) |
| C2—C1—C6—C5 | −0.4 (4) | C38—C39—C40—C35 | −1.2 (7) |
| O6—C1—C6—C5 | −178.2 (3) | C35—O12—C41—C43 | 150.9 (2) |
| C4—C5—C6—C1 | −0.6 (5) | C35—O12—C41—C42 | −109.3 (2) |
| C1—O6—C7—C9 | −88.7 (2) | C43—N3—C42—C44 | −108.3 (2) |
| C1—O6—C7—C8 | 172.60 (19) | C68—N3—C42—C44 | 71.3 (3) |
| C9—N1—C8—C10 | 112.63 (19) | C43—N3—C42—C41 | 8.43 (18) |
| C34—N1—C8—C10 | −69.8 (3) | C68—N3—C42—C41 | −172.0 (3) |
| C9—N1—C8—C7 | −5.46 (17) | O12—C41—C42—N3 | −125.1 (2) |
| C34—N1—C8—C7 | 172.1 (2) | C43—C41—C42—N3 | −7.46 (16) |
| O6—C7—C8—N1 | 125.40 (18) | O12—C41—C42—C44 | −8.3 (3) |
| C9—C7—C8—N1 | 4.78 (15) | C43—C41—C42—C44 | 109.4 (2) |
| O6—C7—C8—C10 | 8.9 (3) | C68—N3—C43—O8 | −6.5 (5) |
| C9—C7—C8—C10 | −111.7 (2) | C42—N3—C43—O8 | 173.1 (3) |
| C34—N1—C9—O2 | 7.3 (4) | C68—N3—C43—C41 | 171.8 (2) |
| C8—N1—C9—O2 | −175.1 (3) | C42—N3—C43—C41 | −8.66 (18) |
| C34—N1—C9—C7 | −172.1 (2) | O12—C41—C43—O8 | −53.8 (4) |
| C8—N1—C9—C7 | 5.54 (18) | C42—C41—C43—O8 | −173.8 (3) |
| O6—C7—C9—O2 | 60.6 (4) | O12—C41—C43—N3 | 128.0 (2) |
| C8—C7—C9—O2 | 175.5 (3) | C42—C41—C43—N3 | 8.07 (17) |
| O6—C7—C9—N1 | −120.1 (2) | N3—C42—C44—C45 | 15.0 (3) |
| C8—C7—C9—N1 | −5.19 (16) | C41—C42—C44—C45 | −83.2 (3) |
| N1—C8—C10—C11 | −18.3 (3) | N3—C42—C44—C49 | −168.2 (2) |
| C7—C8—C10—C11 | 80.8 (3) | C41—C42—C44—C49 | 93.5 (3) |
| N1—C8—C10—C15 | 163.82 (19) | C49—C44—C45—C46 | 0.9 (4) |
| C7—C8—C10—C15 | −97.1 (2) | C42—C44—C45—C46 | 177.6 (2) |
| C15—C10—C11—C12 | −0.7 (4) | C44—C45—C46—C47 | 2.0 (4) |
| C8—C10—C11—C12 | −178.5 (3) | C45—C46—C47—C48 | −3.3 (5) |
| C10—C11—C12—C13 | −1.0 (5) | C46—C47—C48—C49 | 1.7 (5) |
| C11—C12—C13—C14 | 1.1 (6) | C50—O10—C49—C44 | 142.0 (3) |
| C12—C13—C14—C15 | 0.5 (5) | C50—O10—C49—C48 | −42.6 (4) |
| C16—O4—C15—C14 | 32.2 (4) | C45—C44—C49—O10 | 173.0 (2) |
| C16—O4—C15—C10 | −151.8 (2) | C42—C44—C49—O10 | −3.9 (3) |
| C13—C14—C15—O4 | 173.6 (3) | C45—C44—C49—C48 | −2.5 (4) |
| C13—C14—C15—C10 | −2.2 (4) | C42—C44—C49—C48 | −179.4 (2) |
| C11—C10—C15—O4 | −173.8 (2) | C47—C48—C49—O10 | −173.8 (3) |
| C8—C10—C15—O4 | 4.1 (3) | C47—C48—C49—C44 | 1.3 (5) |
| C11—C10—C15—C14 | 2.3 (4) | C49—O10—C50—C51 | −130.4 (3) |
| C8—C10—C15—C14 | −179.8 (2) | C52—O9—C51—C50 | −164.1 (2) |
| C15—O4—C16—C17 | 134.4 (3) | O10—C50—C51—O9 | 66.6 (3) |
| C18—O3—C17—C16 | 153.4 (2) | C51—O9—C52—C53 | −15.0 (4) |
| O4—C16—C17—O3 | −68.4 (3) | C51—O9—C52—C57 | 164.8 (2) |
| C17—O3—C18—C19 | 27.5 (3) | O9—C52—C53—C54 | 179.3 (2) |
| C17—O3—C18—C23 | −154.7 (2) | C57—C52—C53—C54 | −0.5 (4) |
| O3—C18—C19—C20 | 177.7 (2) | C52—C53—C54—C55 | 0.4 (4) |
| C23—C18—C19—C20 | 0.0 (3) | C53—C54—C55—C56 | −0.4 (4) |

| | | | |
|---|---|---|---|
| C18—C19—C20—C21 | −0.2 (3) | C54—C55—C56—C57 | 0.6 (4) |
| C19—C20—C21—C22 | 0.2 (4) | C55—C56—C57—C52 | −0.7 (3) |
| C20—C21—C22—C23 | 0.1 (3) | C55—C56—C57—C58 | 177.1 (2) |
| C21—C22—C23—C18 | −0.2 (3) | O9—C52—C57—C56 | −179.2 (2) |
| C21—C22—C23—C24 | 179.76 (19) | C53—C52—C57—C56 | 0.6 (3) |
| O3—C18—C23—C22 | −177.61 (18) | O9—C52—C57—C58 | 3.0 (3) |
| C19—C18—C23—C22 | 0.2 (3) | C53—C52—C57—C58 | −177.2 (2) |
| O3—C18—C23—C24 | 2.4 (3) | C60—N4—C58—C57 | −106.8 (2) |
| C19—C18—C23—C24 | −179.81 (18) | C67—N4—C58—C57 | 64.9 (3) |
| C26—N2—C24—C23 | 109.9 (2) | C60—N4—C58—C59 | 9.08 (18) |
| C33—N2—C24—C23 | −61.3 (3) | C67—N4—C58—C59 | −179.2 (2) |
| C26—N2—C24—C25 | −7.52 (18) | C56—C57—C58—N4 | 36.9 (3) |
| C33—N2—C24—C25 | −178.7 (2) | C52—C57—C58—N4 | −145.29 (19) |
| C22—C23—C24—N2 | −32.3 (3) | C56—C57—C58—C59 | −60.0 (3) |
| C18—C23—C24—N2 | 147.69 (18) | C52—C57—C58—C59 | 117.8 (2) |
| C22—C23—C24—C25 | 65.7 (3) | C61—O11—C59—C60 | 89.5 (2) |
| C18—C23—C24—C25 | −114.3 (2) | C61—O11—C59—C58 | −171.27 (19) |
| C27—O5—C25—C26 | −85.4 (2) | N4—C58—C59—O11 | −129.7 (2) |
| C27—O5—C25—C24 | 176.11 (19) | C57—C58—C59—O11 | −15.1 (3) |
| N2—C24—C25—O5 | 127.13 (19) | N4—C58—C59—C60 | −7.93 (16) |
| C23—C24—C25—O5 | 11.7 (3) | C57—C58—C59—C60 | 106.7 (2) |
| N2—C24—C25—C26 | 6.54 (16) | C67—N4—C60—O7 | −1.0 (5) |
| C23—C24—C25—C26 | −108.9 (2) | C58—N4—C60—O7 | 170.9 (3) |
| C33—N2—C26—O1 | −1.5 (4) | C67—N4—C60—C59 | 178.9 (2) |
| C24—N2—C26—O1 | −173.3 (3) | C58—N4—C60—C59 | −9.21 (18) |
| C33—N2—C26—C25 | 179.4 (2) | O11—C59—C60—O7 | −56.5 (4) |
| C24—N2—C26—C25 | 7.62 (18) | C58—C59—C60—O7 | −171.4 (3) |
| O5—C25—C26—O1 | 59.4 (4) | O11—C59—C60—N4 | 123.5 (2) |
| C24—C25—C26—O1 | 173.8 (3) | C58—C59—C60—N4 | 8.66 (17) |
| O5—C25—C26—N2 | −121.5 (2) | C59—O11—C61—C66 | −40.3 (3) |
| C24—C25—C26—N2 | −7.15 (17) | C59—O11—C61—C62 | 142.4 (2) |
| C25—O5—C27—C32 | 42.8 (3) | C66—C61—C62—C63 | 0.1 (4) |
| C25—O5—C27—C28 | −139.8 (2) | O11—C61—C62—C63 | 177.4 (3) |
| C32—C27—C28—C29 | −0.5 (4) | C61—C62—C63—C64 | −0.1 (5) |
| O5—C27—C28—C29 | −178.0 (3) | C62—C63—C64—C65 | 0.0 (5) |
| C27—C28—C29—C30 | −0.2 (5) | C63—C64—C65—C66 | 0.2 (4) |
| C28—C29—C30—C31 | 0.8 (4) | C62—C61—C66—C65 | 0.1 (4) |
| C29—C30—C31—C32 | −0.7 (4) | O11—C61—C66—C65 | −177.0 (2) |
| C28—C27—C32—C31 | 0.6 (4) | C64—C65—C66—C61 | −0.3 (4) |
| O5—C27—C32—C31 | 177.9 (2) | C60—N4—C67—C68 | −112.9 (3) |
| C30—C31—C32—C27 | 0.0 (4) | C58—N4—C67—C68 | 78.0 (3) |
| C26—N2—C33—C34 | 107.1 (3) | C43—N3—C68—C67 | −112.1 (3) |
| C24—N2—C33—C34 | −84.2 (3) | C42—N3—C68—C67 | 68.5 (4) |
| C9—N1—C34—C33 | 112.5 (3) | N4—C67—C68—N3 | −97.4 (3) |
| C8—N1—C34—C33 | −64.3 (3) | C71—O13—C70—O14 | 2.0 (5) |
| N2—C33—C34—N1 | 95.2 (2) | C71—O13—C70—C69 | −174.3 (4) |
| C41—O12—C35—C40 | 17.9 (4) | C70—O13—C71—C72 | 175.5 (4) |
| C41—O12—C35—C36 | −162.4 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C53—H53···O6 | 0.93 | 2.52 | 3.344 (3) | 147 |
| C2—H2···O2 | 0.93 | 2.42 | 3.250 (3) | 149 |
| C32—H32···O1 | 0.93 | 2.33 | 3.178 (3) | 151 |
| C66—H66···O7 | 0.93 | 2.48 | 3.299 (3) | 147 |