



Crystal structure of *N*-deacetylappaconitine

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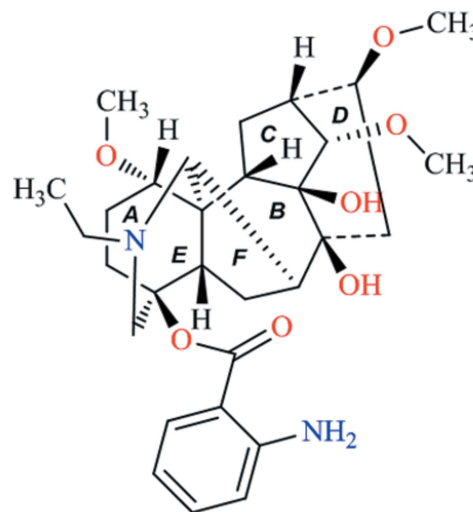
The title compound, $C_{30}H_{42}N_2O_7$ [systematic name: (1*S*,4*S*,5*S*,7*S*,8*S*,9*S*,10*S*,11*S*,13*R*,14*S*,16*S*,17*R*)-20-ethyl-4,8,9-trihydroxy-1,14,16-trimethoxyaconitan-4-yl 2-aminobenzoate], isolated from roots of *Aconitum sinomontanum* Nakai, is a typical aconitane-type C_{19} -diterpenoid alkaloid, which crystallizes with two independent molecules in the asymmetric unit. The conformations of the two independent molecules are closely similar. Each molecule comprises four six-membered rings (*A*, *B*, *D* and *E*) including one six-membered N-containing heterocyclic ring (*E*), and two five-membered rings (*C* and *F*). Rings *A*, *B* and *E* adopt chair conformations, while ring *D* displays a boat conformation. Five-membered rings *C* and *F* exhibit envelope conformations. Intramolecular N—H...O hydrogen bonds between the amino group and carbonyl O atom help to stabilize molecular structure. In the crystal, O—H...O hydrogen bonds link the molecules into zigzag chains propagating in [010].

Keywords: *N*-deacetylappaconitine; C_{19} -diterpenoid alkaloid; O—H...O hydrogen bonding; crystal structure.

CCDC reference: 1409115

1. Related literature

For reviews of typical C_{19} -diterpenoid alkaloids, see: Wang *et al.* (2009, 2010). For the isolation, identification and biological activity of *N*-deacetylappaconitine, see: Peng *et al.* (2000); Romanov *et al.* (2008). For ring numbering, ring conformations and absolute configurations of C_{19} -diterpenoid alkaloids, see: Wang *et al.* (2007); He *et al.* (2008).



2. Experimental

2.1. Crystal data

| | |
|------------------------------|---|
| $C_{30}H_{42}N_2O_7$ | $V = 5525.3(3) \text{ \AA}^3$ |
| $M_r = 542.66$ | $Z = 8$ |
| Orthorhombic, $P2_12_12_1$ | Cu $K\alpha$ radiation |
| $a = 11.7090(3) \text{ \AA}$ | $\mu = 0.75 \text{ mm}^{-1}$ |
| $b = 13.2040(4) \text{ \AA}$ | $T = 173 \text{ K}$ |
| $c = 35.7380(9) \text{ \AA}$ | $0.30 \times 0.30 \times 0.30 \text{ mm}$ |

2.2. Data collection

| | |
|---|--|
| Bruker SMART CCD area-detector diffractometer | 18595 measured reflections |
| Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2002) | 8477 independent reflections |
| $T_{\min} = 0.806$, $T_{\max} = 0.806$ | 7744 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.030$ |

2.3. Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.042$ | 713 parameters |
| $wR(F^2) = 0.111$ | H-atom parameters constrained |
| $S = 1.02$ | $\Delta\rho_{\text{max}} = 0.26 \text{ e \AA}^{-3}$ |
| 8477 reflections | $\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$ |

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------|-------|-------------|-------------|---------------|
| O14—H14A...O6 ⁱ | 0.98 | 2.27 | 2.927 (2) | 123 |
| O11—H11...O12 | 0.84 | 2.40 | 2.944 (2) | 124 |
| O4—H4...O5 | 0.84 | 2.33 | 2.914 (3) | 127 |
| O3—H3...O13 ⁱⁱ | 0.84 | 2.41 | 3.095 (2) | 139 |
| N3—H3D...O8 | 0.91 | 2.02 | 2.687 (3) | 129 |
| N1—H1A...O1 | 0.91 | 2.02 | 2.752 (4) | 137 |

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT*; data reduction: *SAINT* (Bruker, 2002); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXTL*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: CV5490).

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supporting information

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Crystal structure of *N*-deacetylappaconitine

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S1. Comment

The title compound, *N*-deacetylappaconitine, is produced by several species of the plant genus *Aconitum* (*A. sinomontanum*, *A. barbatum*, *A. septentrionale*, *A. leucostomum*, *A. orientale*) and its structure was confirmed by the NMR and MS data. It possesses antiarrhythmic, analgesic, local anesthetic, sedative and anti-inflammatory activity (Peng *et al.* 2000; Wang *et al.* 2009, 2010; Romanov *et al.* 2008). Herewith we present the crystal structure of *N*-deacetylappaconitine (I).

The title compound (I) crystallizes with two independent molecules in the asymmetric unit (Fig. 1). The conformations of both molecules are close (Fig. 2) due to intramolecular N—H \cdots O and O—H \cdots O hydrogen bonds (Table 1). Each molecule is composed from six rings labelled as *A–F* (Wang *et al.*, 2007). Six-membered rings *A* (C1–C5/C11) and *B* (C7–C11/C17) adopt chair conformations; six-membered N-containing heterocyclic ring *E* (C4/C5/C11/C17/N2/C18) display the same chair conformation; the five-membered rings *C* (C9/C10/C12/C13/C14) and *F* (C5/C6/C7/C17/C11) form envelope conformations, in which, atoms C13 and C17, respectively, play the role of flap. The six-membered ring *D* (C8/C9/C14/C13/C16/C15) is in a boat conformation.

In the crystal, intermolecular O—H \cdots O hydrogen bonds (Table 1) link the molecules into zigzag chains propagated in [010].

S2. Experimental

The title compound was isolated from the roots of *Aconitum sinomontanum* Nakai following the known procedure (Peng *et al.*, 2000). Colourless single crystals suitable for X-ray diffraction were obtained by slow evaporation from a methanol solution for two weeks at the room temperature.

S3. Refinement

The hydrogen atoms were placed in calculated positions and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5 U_{\text{eq}}(\text{C}, \text{O})$. The positions of methyl and hydroxy hydrogens were rotationally optimized. In spite of acceptable value of Flack parameter of $-0.07(15)$ in the absence of anomalous scatterers, the absolute configuration of the title compound has been assigned to be the same as that reported for typical natural aconitane-type C_{19} -diterpenoid alkaloids (Wang *et al.*, 2007; He *et al.*, 2008).

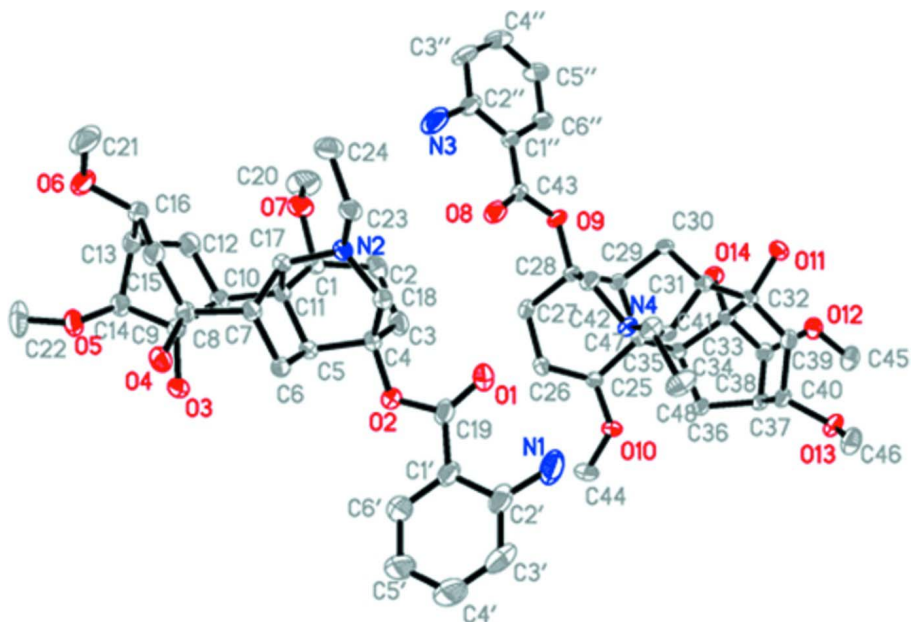


Figure 1

Two independent molecules in the asymmetric unit showing the atomic labeling and 30% probability displacement ellipsoids. H atoms omitted for clarity.

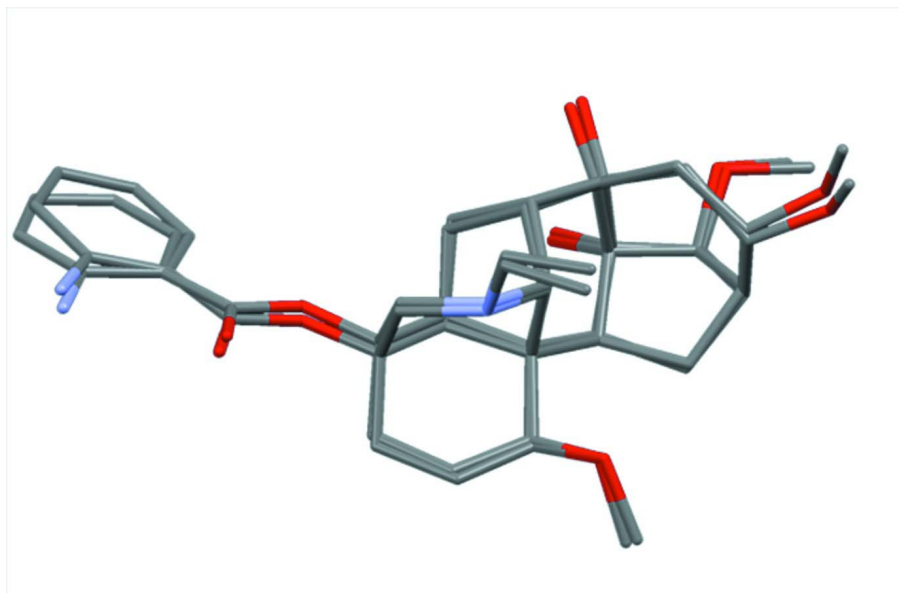


Figure 2

The overlay of two independent molecules.

(I)

Crystal data

$C_{30}H_{42}N_2O_7$

$M_r = 542.66$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 11.7090 (3) \text{ \AA}$

$b = 13.2040 (4) \text{ \AA}$

$c = 35.7380$ (9) Å
 $V = 5525.3$ (3) Å³
 $Z = 8$
 $F(000) = 2336$
 $D_x = 1.305$ Mg m⁻³
 Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 7732 reflections
 $\theta = 3.6\text{--}66.9^\circ$
 $\mu = 0.75$ mm⁻¹
 $T = 173$ K
 Prism, colourless
 $0.30 \times 0.30 \times 0.30$ mm

Data collection

Bruker SMART CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 phi and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2002)
 $T_{\min} = 0.806$, $T_{\max} = 0.806$

18595 measured reflections
 8477 independent reflections
 7744 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$
 $\theta_{\max} = 65.0^\circ$, $\theta_{\min} = 2.5^\circ$
 $h = -13 \rightarrow 13$
 $k = -12 \rightarrow 15$
 $l = -42 \rightarrow 38$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.111$
 $S = 1.02$
 8477 reflections
 713 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
 $w = 1/[\sigma^2(F_o^2) + (0.0677P)^2 + 0.5213P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.26$ e Å⁻³
 $\Delta\rho_{\min} = -0.19$ 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 | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|------------|--------------|-------------|----------------------------------|
| C1 | 0.2568 (2) | 0.43649 (19) | 0.54143 (6) | 0.0422 (6) |
| H1 | 0.3404 | 0.4330 | 0.5358 | 0.051* |
| C2 | 0.2385 (2) | 0.3917 (2) | 0.58046 (6) | 0.0505 (6) |
| H2A | 0.3022 | 0.4132 | 0.5968 | 0.061* |
| H2B | 0.1671 | 0.4198 | 0.5911 | 0.061* |
| C3 | 0.2312 (2) | 0.2773 (2) | 0.58093 (7) | 0.0527 (7) |
| H3A | 0.3069 | 0.2479 | 0.5751 | 0.063* |
| H3B | 0.2081 | 0.2538 | 0.6061 | 0.063* |
| C4 | 0.1451 (2) | 0.24306 (19) | 0.55241 (6) | 0.0401 (5) |
| C5 | 0.1853 (2) | 0.26898 (18) | 0.51258 (6) | 0.0359 (5) |

| | | | | |
|------|--------------|--------------|--------------|-------------|
| H5 | 0.2602 | 0.2362 | 0.5067 | 0.043* |
| C6 | 0.0911 (2) | 0.23517 (18) | 0.48488 (6) | 0.0388 (5) |
| H6A | 0.1250 | 0.2038 | 0.4623 | 0.047* |
| H6B | 0.0387 | 0.1860 | 0.4968 | 0.047* |
| C7 | 0.02808 (19) | 0.33336 (18) | 0.47485 (6) | 0.0364 (5) |
| H7 | -0.0564 | 0.3221 | 0.4754 | 0.044* |
| C8 | 0.06474 (19) | 0.37144 (19) | 0.43617 (6) | 0.0380 (5) |
| C9 | 0.19841 (18) | 0.37717 (18) | 0.43412 (6) | 0.0362 (5) |
| C10 | 0.25048 (19) | 0.41825 (18) | 0.47103 (6) | 0.0369 (5) |
| H10 | 0.3308 | 0.3927 | 0.4721 | 0.044* |
| C11 | 0.19213 (18) | 0.38589 (18) | 0.50856 (6) | 0.0342 (5) |
| C12 | 0.2580 (3) | 0.5349 (2) | 0.46378 (7) | 0.0541 (7) |
| H12A | 0.2160 | 0.5725 | 0.4834 | 0.065* |
| H12B | 0.3387 | 0.5574 | 0.4640 | 0.065* |
| C13 | 0.2039 (2) | 0.5545 (2) | 0.42508 (7) | 0.0503 (6) |
| H13 | 0.2413 | 0.6133 | 0.4124 | 0.060* |
| C14 | 0.2339 (2) | 0.4561 (2) | 0.40577 (6) | 0.0454 (6) |
| H14 | 0.3185 | 0.4527 | 0.4022 | 0.054* |
| C15 | 0.0062 (2) | 0.4726 (2) | 0.42595 (7) | 0.0480 (6) |
| H15A | -0.0228 | 0.4664 | 0.4000 | 0.058* |
| H15B | -0.0612 | 0.4803 | 0.4424 | 0.058* |
| C16 | 0.0749 (3) | 0.5707 (2) | 0.42826 (7) | 0.0531 (7) |
| H16 | 0.0586 | 0.6035 | 0.4529 | 0.064* |
| C17 | 0.06348 (18) | 0.40758 (17) | 0.50614 (6) | 0.0336 (5) |
| H17 | 0.0497 | 0.4792 | 0.4982 | 0.040* |
| C18 | 0.0243 (2) | 0.28618 (19) | 0.55827 (7) | 0.0415 (5) |
| H18A | -0.0319 | 0.2410 | 0.5460 | 0.050* |
| H18B | 0.0070 | 0.2875 | 0.5854 | 0.050* |
| C19 | 0.0950 (2) | 0.0736 (2) | 0.57788 (7) | 0.0531 (7) |
| C20 | 0.3107 (4) | 0.6053 (3) | 0.55720 (12) | 0.0920 (12) |
| H20A | 0.3241 | 0.5891 | 0.5836 | 0.138* |
| H20B | 0.2859 | 0.6760 | 0.5550 | 0.138* |
| H20C | 0.3814 | 0.5956 | 0.5430 | 0.138* |
| C21 | -0.0699 (4) | 0.6774 (3) | 0.40392 (12) | 0.1110 (17) |
| H21A | -0.1243 | 0.6210 | 0.4037 | 0.167* |
| H21B | -0.0878 | 0.7241 | 0.3834 | 0.167* |
| H21C | -0.0751 | 0.7133 | 0.4278 | 0.167* |
| C22 | 0.2309 (3) | 0.4802 (3) | 0.34001 (8) | 0.0855 (11) |
| H22A | 0.2215 | 0.5538 | 0.3417 | 0.128* |
| H22B | 0.1949 | 0.4556 | 0.3170 | 0.128* |
| H22C | 0.3124 | 0.4635 | 0.3396 | 0.128* |
| C23 | -0.1048 (2) | 0.4258 (2) | 0.54681 (7) | 0.0426 (5) |
| H23A | -0.1374 | 0.4002 | 0.5706 | 0.051* |
| H23B | -0.1514 | 0.3981 | 0.5261 | 0.051* |
| C24 | -0.1135 (3) | 0.5397 (2) | 0.54635 (9) | 0.0624 (8) |
| H24A | -0.0592 | 0.5682 | 0.5644 | 0.094* |
| H24B | -0.1912 | 0.5600 | 0.5532 | 0.094* |
| H24C | -0.0957 | 0.5648 | 0.5212 | 0.094* |

| | | | | |
|------|--------------|---------------|-------------|------------|
| C25 | 0.39217 (18) | 0.08850 (16) | 0.71788 (6) | 0.0320 (5) |
| H25 | 0.4767 | 0.0942 | 0.7212 | 0.038* |
| C26 | 0.3616 (2) | 0.14105 (18) | 0.68090 (6) | 0.0408 (5) |
| H26A | 0.4200 | 0.1237 | 0.6619 | 0.049* |
| H26B | 0.2873 | 0.1148 | 0.6720 | 0.049* |
| C27 | 0.3544 (2) | 0.25473 (18) | 0.68429 (6) | 0.0399 (5) |
| H27A | 0.3261 | 0.2841 | 0.6605 | 0.048* |
| H27B | 0.4311 | 0.2831 | 0.6894 | 0.048* |
| C28 | 0.27342 (18) | 0.28149 (16) | 0.71598 (6) | 0.0313 (5) |
| C29 | 0.32419 (18) | 0.24848 (16) | 0.75345 (6) | 0.0309 (4) |
| H29 | 0.3994 | 0.2820 | 0.7582 | 0.037* |
| C30 | 0.2373 (2) | 0.27287 (16) | 0.78494 (6) | 0.0364 (5) |
| H30A | 0.2768 | 0.3006 | 0.8072 | 0.044* |
| H30B | 0.1802 | 0.3228 | 0.7762 | 0.044* |
| C31 | 0.18008 (18) | 0.17164 (16) | 0.79424 (6) | 0.0334 (5) |
| H31 | 0.0956 | 0.1804 | 0.7967 | 0.040* |
| C32 | 0.22999 (19) | 0.12554 (17) | 0.83008 (6) | 0.0350 (5) |
| C33 | 0.36444 (19) | 0.12486 (17) | 0.82810 (6) | 0.0338 (5) |
| C34 | 0.40731 (17) | 0.09500 (16) | 0.78846 (6) | 0.0312 (4) |
| H34 | 0.4846 | 0.1263 | 0.7856 | 0.037* |
| C35 | 0.33562 (16) | 0.13118 (15) | 0.75396 (5) | 0.0272 (4) |
| C36 | 0.42728 (19) | -0.02177 (18) | 0.79183 (6) | 0.0383 (5) |
| H36A | 0.3865 | -0.0580 | 0.7716 | 0.046* |
| H36B | 0.5097 | -0.0376 | 0.7900 | 0.046* |
| C37 | 0.38056 (19) | -0.05397 (17) | 0.83042 (6) | 0.0361 (5) |
| H37 | 0.4222 | -0.1147 | 0.8401 | 0.043* |
| C38 | 0.41089 (19) | 0.03980 (18) | 0.85266 (6) | 0.0369 (5) |
| H38 | 0.4959 | 0.0458 | 0.8539 | 0.044* |
| C39 | 0.17956 (19) | 0.01971 (18) | 0.83848 (6) | 0.0391 (5) |
| H39A | 0.1624 | 0.0166 | 0.8656 | 0.047* |
| H39B | 0.1059 | 0.0142 | 0.8250 | 0.047* |
| C40 | 0.2514 (2) | -0.07378 (17) | 0.82849 (6) | 0.0366 (5) |
| H40 | 0.2319 | -0.0947 | 0.8024 | 0.044* |
| C41 | 0.20902 (16) | 0.10515 (16) | 0.75957 (6) | 0.0284 (4) |
| H41 | 0.1999 | 0.0317 | 0.7657 | 0.034* |
| C42 | 0.15309 (19) | 0.23520 (17) | 0.71190 (6) | 0.0367 (5) |
| H42A | 0.0981 | 0.2770 | 0.7262 | 0.044* |
| H42B | 0.1304 | 0.2374 | 0.6852 | 0.044* |
| C43 | 0.21456 (19) | 0.45045 (17) | 0.69410 (6) | 0.0368 (5) |
| C44 | 0.4515 (3) | -0.0713 (2) | 0.69438 (9) | 0.0706 (9) |
| H44A | 0.4605 | -0.0428 | 0.6692 | 0.106* |
| H44B | 0.4286 | -0.1425 | 0.6924 | 0.106* |
| H44C | 0.5242 | -0.0667 | 0.7079 | 0.106* |
| C45 | 0.4057 (3) | -0.0248 (2) | 0.91444 (7) | 0.0575 (7) |
| H45A | 0.3667 | -0.0890 | 0.9092 | 0.086* |
| H45B | 0.3901 | -0.0041 | 0.9403 | 0.086* |
| H45C | 0.4882 | -0.0337 | 0.9110 | 0.086* |
| C46 | 0.1203 (2) | -0.2031 (2) | 0.84451 (8) | 0.0578 (7) |

| | | | | |
|------|--------------|--------------|--------------|-------------|
| H46A | 0.0578 | -0.1553 | 0.8490 | 0.087* |
| H46B | 0.1102 | -0.2630 | 0.8604 | 0.087* |
| H46C | 0.1200 | -0.2236 | 0.8182 | 0.087* |
| C47 | 0.02761 (19) | 0.09681 (19) | 0.72501 (7) | 0.0428 (6) |
| H47A | -0.0084 | 0.1189 | 0.7013 | 0.051* |
| H47B | -0.0132 | 0.1307 | 0.7458 | 0.051* |
| C48 | 0.0124 (2) | -0.0161 (2) | 0.72891 (10) | 0.0645 (8) |
| H48A | 0.0617 | -0.0509 | 0.7109 | 0.097* |
| H48B | -0.0675 | -0.0339 | 0.7241 | 0.097* |
| H48C | 0.0332 | -0.0368 | 0.7543 | 0.097* |
| C1' | 0.0897 (2) | -0.0336 (2) | 0.56605 (8) | 0.0553 (7) |
| C2' | 0.0381 (2) | -0.1087 (3) | 0.58835 (9) | 0.0642 (8) |
| C3' | 0.0275 (3) | -0.2063 (3) | 0.57384 (13) | 0.0817 (11) |
| H3' | -0.0092 | -0.2571 | 0.5883 | 0.098* |
| C4' | 0.0689 (4) | -0.2303 (3) | 0.53928 (13) | 0.0997 (14) |
| H4' | 0.0612 | -0.2974 | 0.5300 | 0.120* |
| C5' | 0.1214 (5) | -0.1580 (3) | 0.51803 (12) | 0.1061 (15) |
| H5' | 0.1517 | -0.1752 | 0.4942 | 0.127* |
| C6' | 0.1303 (4) | -0.0612 (3) | 0.53097 (9) | 0.0766 (10) |
| H6' | 0.1653 | -0.0114 | 0.5156 | 0.092* |
| C1'' | 0.22222 (19) | 0.55868 (17) | 0.70302 (6) | 0.0365 (5) |
| C2'' | 0.1771 (3) | 0.6321 (2) | 0.67866 (8) | 0.0542 (7) |
| C3'' | 0.1854 (3) | 0.7340 (2) | 0.68911 (10) | 0.0672 (9) |
| H3'' | 0.1571 | 0.7846 | 0.6727 | 0.081* |
| C4'' | 0.2335 (3) | 0.7625 (2) | 0.72248 (10) | 0.0643 (8) |
| H4'' | 0.2361 | 0.8321 | 0.7292 | 0.077* |
| C5'' | 0.2778 (2) | 0.6908 (2) | 0.74615 (8) | 0.0548 (7) |
| H5'' | 0.3122 | 0.7106 | 0.7691 | 0.066* |
| C6'' | 0.2721 (2) | 0.59137 (19) | 0.73669 (7) | 0.0429 (5) |
| H6'' | 0.3029 | 0.5424 | 0.7533 | 0.051* |
| N1 | -0.0034 (3) | -0.0889 (3) | 0.62340 (8) | 0.0928 (10) |
| H1A | 0.0242 | -0.0281 | 0.6312 | 0.111* |
| H1B | 0.0201 | -0.1384 | 0.6394 | 0.111* |
| N2 | 0.01194 (16) | 0.38839 (15) | 0.54309 (5) | 0.0373 (4) |
| N3 | 0.1290 (3) | 0.6066 (2) | 0.64485 (7) | 0.0889 (10) |
| H3C | 0.0735 | 0.6526 | 0.6394 | 0.107* |
| H3D | 0.0974 | 0.5438 | 0.6467 | 0.107* |
| N4 | 0.14633 (14) | 0.13030 (14) | 0.72516 (5) | 0.0328 (4) |
| O1 | 0.0612 (2) | 0.10686 (18) | 0.60764 (5) | 0.0740 (6) |
| O2 | 0.14170 (17) | 0.13201 (13) | 0.55120 (4) | 0.0500 (4) |
| O3 | 0.24945 (15) | 0.28229 (13) | 0.42563 (4) | 0.0443 (4) |
| H3 | 0.2200 | 0.2586 | 0.4061 | 0.066* |
| O4 | 0.02651 (16) | 0.29539 (14) | 0.41009 (5) | 0.0487 (4) |
| H4 | 0.0438 | 0.3130 | 0.3882 | 0.073* |
| O5 | 0.17912 (16) | 0.43398 (15) | 0.37103 (4) | 0.0538 (5) |
| O6 | 0.0426 (2) | 0.63931 (16) | 0.39921 (6) | 0.0710 (6) |
| O7 | 0.22516 (17) | 0.54113 (14) | 0.54284 (5) | 0.0554 (5) |
| O8 | 0.16607 (18) | 0.41487 (13) | 0.66696 (5) | 0.0538 (5) |

| | | | | |
|------|--------------|---------------|-------------|------------|
| O9 | 0.26648 (14) | 0.39190 (11) | 0.71983 (4) | 0.0373 (3) |
| O10 | 0.36612 (14) | -0.01612 (12) | 0.71417 (4) | 0.0407 (4) |
| O11 | 0.19519 (16) | 0.19342 (13) | 0.85988 (4) | 0.0490 (4) |
| H11 | 0.2113 | 0.1673 | 0.8806 | 0.059* |
| O12 | 0.36556 (16) | 0.05052 (14) | 0.88956 (4) | 0.0481 (4) |
| O13 | 0.22545 (14) | -0.15629 (13) | 0.85308 (4) | 0.0448 (4) |
| O14 | 0.41392 (15) | 0.21944 (12) | 0.83770 (4) | 0.0441 (4) |
| H14A | 0.3753 | 0.2467 | 0.8599 | 0.053* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C1 | 0.0410 (12) | 0.0460 (14) | 0.0396 (12) | -0.0053 (11) | -0.0029 (10) | -0.0089 (11) |
| C2 | 0.0540 (14) | 0.0645 (18) | 0.0329 (12) | -0.0067 (14) | -0.0057 (11) | -0.0124 (12) |
| C3 | 0.0592 (15) | 0.0672 (19) | 0.0317 (12) | 0.0090 (14) | -0.0042 (11) | 0.0023 (12) |
| C4 | 0.0501 (13) | 0.0397 (14) | 0.0304 (11) | 0.0055 (11) | 0.0030 (10) | 0.0013 (10) |
| C5 | 0.0430 (11) | 0.0346 (13) | 0.0300 (10) | 0.0044 (10) | 0.0022 (9) | -0.0028 (9) |
| C6 | 0.0528 (13) | 0.0309 (12) | 0.0328 (11) | -0.0056 (11) | 0.0021 (10) | -0.0010 (9) |
| C7 | 0.0375 (11) | 0.0377 (13) | 0.0339 (11) | -0.0049 (10) | 0.0020 (9) | -0.0020 (10) |
| C8 | 0.0419 (12) | 0.0401 (14) | 0.0319 (11) | 0.0001 (10) | -0.0036 (9) | 0.0001 (10) |
| C9 | 0.0404 (11) | 0.0365 (13) | 0.0318 (11) | 0.0025 (10) | 0.0049 (9) | -0.0010 (9) |
| C10 | 0.0363 (11) | 0.0398 (13) | 0.0346 (11) | -0.0016 (10) | 0.0037 (9) | -0.0031 (10) |
| C11 | 0.0359 (10) | 0.0376 (13) | 0.0290 (10) | 0.0020 (10) | 0.0004 (9) | -0.0028 (9) |
| C12 | 0.0649 (16) | 0.0497 (16) | 0.0476 (14) | -0.0161 (14) | 0.0096 (13) | -0.0014 (13) |
| C13 | 0.0678 (16) | 0.0390 (14) | 0.0440 (13) | -0.0073 (13) | 0.0152 (12) | 0.0097 (11) |
| C14 | 0.0482 (12) | 0.0507 (15) | 0.0373 (12) | 0.0017 (12) | 0.0070 (10) | 0.0046 (11) |
| C15 | 0.0514 (13) | 0.0521 (16) | 0.0403 (13) | 0.0120 (12) | 0.0034 (11) | 0.0064 (12) |
| C16 | 0.0776 (18) | 0.0401 (14) | 0.0415 (13) | 0.0126 (14) | 0.0174 (13) | 0.0076 (11) |
| C17 | 0.0403 (11) | 0.0304 (12) | 0.0302 (10) | 0.0013 (9) | 0.0027 (9) | -0.0005 (9) |
| C18 | 0.0490 (13) | 0.0394 (14) | 0.0359 (12) | 0.0039 (11) | 0.0088 (10) | 0.0037 (10) |
| C19 | 0.0596 (15) | 0.0547 (17) | 0.0449 (14) | 0.0114 (14) | 0.0035 (12) | 0.0175 (13) |
| C20 | 0.107 (3) | 0.060 (2) | 0.109 (3) | -0.020 (2) | -0.031 (2) | -0.026 (2) |
| C21 | 0.126 (3) | 0.095 (3) | 0.112 (3) | 0.070 (3) | 0.051 (3) | 0.049 (3) |
| C22 | 0.096 (2) | 0.120 (3) | 0.0402 (15) | 0.004 (2) | 0.0096 (16) | 0.0289 (18) |
| C23 | 0.0408 (11) | 0.0427 (14) | 0.0443 (12) | -0.0018 (11) | 0.0094 (10) | -0.0046 (11) |
| C24 | 0.0607 (16) | 0.0464 (17) | 0.080 (2) | 0.0064 (14) | 0.0222 (15) | -0.0036 (15) |
| C25 | 0.0344 (10) | 0.0266 (11) | 0.0352 (11) | -0.0008 (9) | 0.0069 (9) | -0.0022 (9) |
| C26 | 0.0531 (13) | 0.0394 (13) | 0.0300 (11) | -0.0009 (11) | 0.0092 (10) | -0.0009 (10) |
| C27 | 0.0517 (13) | 0.0338 (13) | 0.0341 (11) | -0.0029 (11) | 0.0052 (10) | 0.0083 (10) |
| C28 | 0.0401 (11) | 0.0230 (11) | 0.0309 (10) | -0.0018 (9) | -0.0039 (9) | 0.0014 (8) |
| C29 | 0.0367 (10) | 0.0242 (11) | 0.0317 (10) | -0.0015 (9) | -0.0028 (9) | -0.0022 (9) |
| C30 | 0.0543 (13) | 0.0243 (11) | 0.0308 (10) | 0.0111 (10) | -0.0008 (10) | -0.0002 (9) |
| C31 | 0.0354 (10) | 0.0297 (12) | 0.0351 (11) | 0.0092 (9) | 0.0042 (9) | 0.0005 (9) |
| C32 | 0.0416 (11) | 0.0325 (12) | 0.0309 (10) | 0.0075 (10) | 0.0079 (9) | 0.0010 (9) |
| C33 | 0.0409 (11) | 0.0282 (12) | 0.0324 (11) | -0.0012 (10) | -0.0019 (9) | -0.0016 (9) |
| C34 | 0.0307 (9) | 0.0291 (12) | 0.0338 (11) | 0.0006 (9) | 0.0024 (8) | 0.0009 (9) |
| C35 | 0.0304 (9) | 0.0233 (11) | 0.0278 (10) | -0.0007 (8) | 0.0010 (8) | -0.0006 (8) |
| C36 | 0.0427 (11) | 0.0337 (12) | 0.0386 (12) | 0.0092 (10) | 0.0065 (10) | 0.0072 (10) |

| | | | | | | |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| C37 | 0.0418 (12) | 0.0299 (12) | 0.0367 (11) | 0.0070 (10) | 0.0006 (9) | 0.0087 (9) |
| C38 | 0.0355 (10) | 0.0406 (13) | 0.0347 (11) | 0.0011 (10) | -0.0011 (9) | 0.0046 (10) |
| C39 | 0.0363 (10) | 0.0428 (14) | 0.0382 (12) | 0.0029 (10) | 0.0061 (9) | 0.0104 (10) |
| C40 | 0.0452 (12) | 0.0309 (12) | 0.0337 (11) | -0.0005 (10) | -0.0017 (9) | 0.0065 (9) |
| C41 | 0.0306 (10) | 0.0224 (10) | 0.0323 (10) | 0.0010 (8) | 0.0027 (8) | 0.0026 (8) |
| C42 | 0.0416 (11) | 0.0313 (12) | 0.0372 (11) | 0.0007 (10) | -0.0066 (9) | 0.0037 (10) |
| C43 | 0.0458 (12) | 0.0311 (12) | 0.0335 (11) | -0.0012 (10) | 0.0023 (9) | 0.0058 (9) |
| C44 | 0.098 (2) | 0.0424 (16) | 0.0711 (19) | 0.0198 (17) | 0.0277 (18) | -0.0096 (14) |
| C45 | 0.0682 (16) | 0.0618 (18) | 0.0424 (13) | 0.0017 (15) | -0.0074 (12) | 0.0179 (13) |
| C46 | 0.0608 (16) | 0.0573 (18) | 0.0553 (15) | -0.0205 (15) | -0.0011 (13) | 0.0116 (13) |
| C47 | 0.0357 (11) | 0.0384 (14) | 0.0543 (14) | -0.0030 (10) | -0.0076 (10) | 0.0064 (11) |
| C48 | 0.0518 (15) | 0.0461 (17) | 0.095 (2) | -0.0143 (13) | -0.0165 (15) | 0.0080 (16) |
| C1' | 0.0630 (15) | 0.0443 (16) | 0.0587 (16) | 0.0072 (14) | 0.0055 (13) | 0.0178 (13) |
| C2' | 0.0569 (15) | 0.064 (2) | 0.0711 (19) | 0.0147 (16) | 0.0082 (14) | 0.0300 (16) |
| C3' | 0.078 (2) | 0.049 (2) | 0.118 (3) | -0.0027 (17) | 0.004 (2) | 0.032 (2) |
| C4' | 0.128 (4) | 0.054 (2) | 0.117 (3) | -0.021 (2) | 0.021 (3) | -0.001 (2) |
| C5' | 0.168 (4) | 0.050 (2) | 0.101 (3) | -0.022 (3) | 0.044 (3) | -0.010 (2) |
| C6' | 0.106 (3) | 0.054 (2) | 0.070 (2) | -0.010 (2) | 0.0229 (19) | 0.0025 (16) |
| C1'' | 0.0412 (11) | 0.0269 (12) | 0.0413 (12) | 0.0021 (10) | 0.0055 (10) | 0.0039 (9) |
| C2'' | 0.0719 (17) | 0.0382 (15) | 0.0524 (15) | 0.0052 (14) | -0.0059 (13) | 0.0087 (12) |
| C3'' | 0.089 (2) | 0.0286 (14) | 0.083 (2) | 0.0108 (15) | -0.0110 (18) | 0.0108 (14) |
| C4'' | 0.0712 (18) | 0.0291 (14) | 0.093 (2) | 0.0004 (14) | -0.0004 (17) | -0.0093 (15) |
| C5'' | 0.0589 (15) | 0.0367 (14) | 0.0689 (17) | -0.0007 (13) | -0.0072 (14) | -0.0109 (13) |
| C6'' | 0.0450 (12) | 0.0373 (14) | 0.0463 (13) | 0.0005 (11) | 0.0011 (10) | -0.0011 (11) |
| N1 | 0.115 (2) | 0.087 (2) | 0.0763 (19) | 0.014 (2) | 0.0178 (18) | 0.0409 (18) |
| N2 | 0.0414 (10) | 0.0371 (11) | 0.0335 (9) | 0.0000 (9) | 0.0076 (8) | -0.0006 (8) |
| N3 | 0.145 (3) | 0.0551 (16) | 0.0664 (16) | 0.0170 (19) | -0.0368 (18) | 0.0142 (14) |
| N4 | 0.0334 (8) | 0.0272 (10) | 0.0378 (9) | -0.0026 (8) | -0.0044 (7) | 0.0050 (8) |
| O1 | 0.1100 (17) | 0.0679 (14) | 0.0440 (10) | 0.0173 (14) | 0.0202 (11) | 0.0133 (10) |
| O2 | 0.0732 (11) | 0.0378 (10) | 0.0391 (9) | 0.0081 (9) | 0.0077 (8) | 0.0060 (7) |
| O3 | 0.0529 (9) | 0.0415 (10) | 0.0384 (8) | 0.0108 (8) | 0.0026 (7) | -0.0044 (7) |
| O4 | 0.0586 (10) | 0.0535 (11) | 0.0339 (8) | -0.0027 (9) | -0.0060 (8) | -0.0057 (8) |
| O5 | 0.0633 (11) | 0.0652 (12) | 0.0329 (8) | 0.0044 (10) | 0.0075 (8) | 0.0056 (8) |
| O6 | 0.0880 (14) | 0.0576 (13) | 0.0673 (12) | 0.0311 (12) | 0.0275 (11) | 0.0269 (10) |
| O7 | 0.0685 (11) | 0.0434 (11) | 0.0543 (10) | -0.0052 (9) | -0.0096 (9) | -0.0171 (9) |
| O8 | 0.0842 (13) | 0.0365 (9) | 0.0406 (9) | 0.0002 (9) | -0.0173 (9) | 0.0018 (8) |
| O9 | 0.0536 (9) | 0.0210 (7) | 0.0374 (8) | 0.0001 (7) | -0.0058 (7) | 0.0033 (6) |
| O10 | 0.0546 (9) | 0.0263 (8) | 0.0411 (8) | 0.0031 (7) | 0.0062 (8) | -0.0068 (7) |
| O11 | 0.0695 (11) | 0.0457 (10) | 0.0319 (8) | 0.0154 (9) | 0.0094 (8) | -0.0014 (7) |
| O12 | 0.0626 (10) | 0.0508 (11) | 0.0309 (8) | 0.0075 (9) | -0.0024 (7) | 0.0074 (7) |
| O13 | 0.0534 (9) | 0.0359 (9) | 0.0452 (9) | -0.0099 (8) | -0.0054 (8) | 0.0136 (7) |
| O14 | 0.0593 (10) | 0.0344 (9) | 0.0387 (8) | -0.0057 (8) | -0.0036 (8) | -0.0029 (7) |

Geometric parameters (Å, °)

| | | | |
|--------|-----------|----------|-----------|
| C1—O7 | 1.431 (3) | C29—H29 | 1.0000 |
| C1—C2 | 1.530 (3) | C30—C31 | 1.532 (3) |
| C1—C11 | 1.549 (3) | C30—H30A | 0.9900 |

| | | | |
|----------|-----------|----------|-----------|
| C1—H1 | 1.0000 | C30—H30B | 0.9900 |
| C2—C3 | 1.512 (4) | C31—C32 | 1.534 (3) |
| C2—H2A | 0.9900 | C31—C41 | 1.556 (3) |
| C2—H2B | 0.9900 | C31—H31 | 1.0000 |
| C3—C4 | 1.504 (3) | C32—O11 | 1.450 (3) |
| C3—H3A | 0.9900 | C32—C39 | 1.546 (3) |
| C3—H3B | 0.9900 | C32—C33 | 1.576 (3) |
| C4—O2 | 1.467 (3) | C33—O14 | 1.419 (3) |
| C4—C5 | 1.538 (3) | C33—C38 | 1.526 (3) |
| C4—C18 | 1.539 (3) | C33—C34 | 1.554 (3) |
| C5—C6 | 1.548 (3) | C34—C36 | 1.564 (3) |
| C5—C11 | 1.552 (3) | C34—C35 | 1.566 (3) |
| C5—H5 | 1.0000 | C34—H34 | 1.0000 |
| C6—C7 | 1.534 (3) | C35—C41 | 1.535 (3) |
| C6—H6A | 0.9900 | C36—C37 | 1.543 (3) |
| C6—H6B | 0.9900 | C36—H36A | 0.9900 |
| C7—C8 | 1.532 (3) | C36—H36B | 0.9900 |
| C7—C17 | 1.544 (3) | C37—C38 | 1.514 (3) |
| C7—H7 | 1.0000 | C37—C40 | 1.536 (3) |
| C8—O4 | 1.441 (3) | C37—H37 | 1.0000 |
| C8—C15 | 1.546 (3) | C38—O12 | 1.429 (3) |
| C8—C9 | 1.569 (3) | C38—H38 | 1.0000 |
| C9—O3 | 1.421 (3) | C39—C40 | 1.536 (3) |
| C9—C14 | 1.511 (3) | C39—H39A | 0.9900 |
| C9—C10 | 1.551 (3) | C39—H39B | 0.9900 |
| C10—C12 | 1.565 (3) | C40—O13 | 1.432 (3) |
| C10—C11 | 1.565 (3) | C40—H40 | 1.0000 |
| C10—H10 | 1.0000 | C41—N4 | 1.470 (3) |
| C11—C17 | 1.536 (3) | C41—H41 | 1.0000 |
| C12—C13 | 1.543 (4) | C42—N4 | 1.466 (3) |
| C12—H12A | 0.9900 | C42—H42A | 0.9900 |
| C12—H12B | 0.9900 | C42—H42B | 0.9900 |
| C13—C14 | 1.513 (4) | C43—O8 | 1.218 (3) |
| C13—C16 | 1.530 (4) | C43—O9 | 1.346 (3) |
| C13—H13 | 1.0000 | C43—C1'' | 1.467 (3) |
| C14—O5 | 1.427 (3) | C44—O10 | 1.425 (3) |
| C14—H14 | 1.0000 | C44—H44A | 0.9800 |
| C15—C16 | 1.526 (4) | C44—H44B | 0.9800 |
| C15—H15A | 0.9900 | C44—H44C | 0.9800 |
| C15—H15B | 0.9900 | C45—O12 | 1.415 (3) |
| C16—O6 | 1.429 (3) | C45—H45A | 0.9800 |
| C16—H16 | 1.0000 | C45—H45B | 0.9800 |
| C17—N2 | 1.474 (3) | C45—H45C | 0.9800 |
| C17—H17 | 1.0000 | C46—O13 | 1.411 (3) |
| C18—N2 | 1.462 (3) | C46—H46A | 0.9800 |
| C18—H18A | 0.9900 | C46—H46B | 0.9800 |
| C18—H18B | 0.9900 | C46—H46C | 0.9800 |
| C19—O1 | 1.217 (3) | C47—N4 | 1.459 (3) |

| | | | |
|-----------|-------------|---------------|-------------|
| C19—O2 | 1.343 (3) | C47—C48 | 1.507 (4) |
| C19—C1' | 1.478 (4) | C47—H47A | 0.9900 |
| C20—O7 | 1.409 (4) | C47—H47B | 0.9900 |
| C20—H20A | 0.9800 | C48—H48A | 0.9800 |
| C20—H20B | 0.9800 | C48—H48B | 0.9800 |
| C20—H20C | 0.9800 | C48—H48C | 0.9800 |
| C21—O6 | 1.419 (4) | C1'—C6' | 1.390 (4) |
| C21—H21A | 0.9800 | C1'—C2' | 1.408 (4) |
| C21—H21B | 0.9800 | C2'—N1 | 1.368 (4) |
| C21—H21C | 0.9800 | C2'—C3' | 1.395 (5) |
| C22—O5 | 1.403 (3) | C3'—C4' | 1.364 (6) |
| C22—H22A | 0.9800 | C3'—H3' | 0.9500 |
| C22—H22B | 0.9800 | C4'—C5' | 1.366 (5) |
| C22—H22C | 0.9800 | C4'—H4' | 0.9500 |
| C23—N2 | 1.460 (3) | C5'—C6' | 1.363 (5) |
| C23—C24 | 1.508 (4) | C5'—H5' | 0.9500 |
| C23—H23A | 0.9900 | C6'—H6' | 0.9500 |
| C23—H23B | 0.9900 | C1''—C6'' | 1.405 (3) |
| C24—H24A | 0.9800 | C1''—C2'' | 1.406 (3) |
| C24—H24B | 0.9800 | C2''—N3 | 1.375 (4) |
| C24—H24C | 0.9800 | C2''—C3'' | 1.400 (4) |
| C25—O10 | 1.421 (3) | C3''—C4'' | 1.372 (4) |
| C25—C26 | 1.535 (3) | C3''—H3'' | 0.9500 |
| C25—C35 | 1.555 (3) | C4''—C5'' | 1.372 (4) |
| C25—H25 | 1.0000 | C4''—H4'' | 0.9500 |
| C26—C27 | 1.508 (3) | C5''—C6'' | 1.357 (3) |
| C26—H26A | 0.9900 | C5''—H5'' | 0.9500 |
| C26—H26B | 0.9900 | C6''—H6'' | 0.9500 |
| C27—C28 | 1.519 (3) | N1—H1A | 0.9100 |
| C27—H27A | 0.9900 | N1—H1B | 0.9100 |
| C27—H27B | 0.9900 | N3—H3C | 0.9100 |
| C28—O9 | 1.467 (2) | N3—H3D | 0.9100 |
| C28—C29 | 1.528 (3) | O3—H3 | 0.8400 |
| C28—C42 | 1.543 (3) | O4—H4 | 0.8400 |
| C29—C30 | 1.551 (3) | O11—H11 | 0.8400 |
| C29—C35 | 1.555 (3) | O14—H14A | 0.9800 |
| O7—C1—C2 | 107.8 (2) | C31—C30—C29 | 105.27 (17) |
| O7—C1—C11 | 108.43 (19) | C31—C30—H30A | 110.7 |
| C2—C1—C11 | 117.1 (2) | C29—C30—H30A | 110.7 |
| O7—C1—H1 | 107.7 | C31—C30—H30B | 110.7 |
| C2—C1—H1 | 107.7 | C29—C30—H30B | 110.7 |
| C11—C1—H1 | 107.7 | H30A—C30—H30B | 108.8 |
| C3—C2—C1 | 113.8 (2) | C30—C31—C32 | 111.15 (18) |
| C3—C2—H2A | 108.8 | C30—C31—C41 | 102.96 (16) |
| C1—C2—H2A | 108.8 | C32—C31—C41 | 110.98 (16) |
| C3—C2—H2B | 108.8 | C30—C31—H31 | 110.5 |
| C1—C2—H2B | 108.8 | C32—C31—H31 | 110.5 |

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| H2A—C2—H2B | 107.7 | C41—C31—H31 | 110.5 |
| C4—C3—C2 | 109.3 (2) | O11—C32—C31 | 105.12 (17) |
| C4—C3—H3A | 109.8 | O11—C32—C39 | 107.97 (17) |
| C2—C3—H3A | 109.8 | C31—C32—C39 | 112.04 (19) |
| C4—C3—H3B | 109.8 | O11—C32—C33 | 108.49 (19) |
| C2—C3—H3B | 109.8 | C31—C32—C33 | 110.21 (17) |
| H3A—C3—H3B | 108.3 | C39—C32—C33 | 112.65 (18) |
| O2—C4—C3 | 109.8 (2) | O14—C33—C38 | 111.30 (17) |
| O2—C4—C5 | 101.74 (18) | O14—C33—C34 | 108.18 (17) |
| C3—C4—C5 | 110.8 (2) | C38—C33—C34 | 102.86 (17) |
| O2—C4—C18 | 110.4 (2) | O14—C33—C32 | 113.09 (19) |
| C3—C4—C18 | 114.4 (2) | C38—C33—C32 | 109.54 (18) |
| C5—C4—C18 | 108.98 (19) | C34—C33—C32 | 111.41 (17) |
| C4—C5—C6 | 108.03 (19) | C33—C34—C36 | 103.19 (17) |
| C4—C5—C11 | 108.83 (18) | C33—C34—C35 | 117.85 (16) |
| C6—C5—C11 | 105.32 (17) | C36—C34—C35 | 116.19 (18) |
| C4—C5—H5 | 111.5 | C33—C34—H34 | 106.2 |
| C6—C5—H5 | 111.5 | C36—C34—H34 | 106.2 |
| C11—C5—H5 | 111.5 | C35—C34—H34 | 106.2 |
| C7—C6—C5 | 104.39 (17) | C41—C35—C29 | 98.14 (16) |
| C7—C6—H6A | 110.9 | C41—C35—C25 | 116.01 (17) |
| C5—C6—H6A | 110.9 | C29—C35—C25 | 112.82 (16) |
| C7—C6—H6B | 110.9 | C41—C35—C34 | 110.27 (16) |
| C5—C6—H6B | 110.9 | C29—C35—C34 | 111.05 (16) |
| H6A—C6—H6B | 108.9 | C25—C35—C34 | 108.30 (16) |
| C8—C7—C6 | 110.69 (18) | C37—C36—C34 | 106.70 (18) |
| C8—C7—C17 | 111.72 (18) | C37—C36—H36A | 110.4 |
| C6—C7—C17 | 103.77 (17) | C34—C36—H36A | 110.4 |
| C8—C7—H7 | 110.2 | C37—C36—H36B | 110.4 |
| C6—C7—H7 | 110.2 | C34—C36—H36B | 110.4 |
| C17—C7—H7 | 110.2 | H36A—C36—H36B | 108.6 |
| O4—C8—C7 | 105.52 (18) | C38—C37—C40 | 113.19 (19) |
| O4—C8—C15 | 108.17 (18) | C38—C37—C36 | 99.25 (18) |
| C7—C8—C15 | 111.87 (19) | C40—C37—C36 | 110.85 (18) |
| O4—C8—C9 | 108.27 (19) | C38—C37—H37 | 111.0 |
| C7—C8—C9 | 109.72 (18) | C40—C37—H37 | 111.0 |
| C15—C8—C9 | 112.9 (2) | C36—C37—H37 | 111.0 |
| O3—C9—C14 | 110.43 (18) | O12—C38—C37 | 118.60 (19) |
| O3—C9—C10 | 108.94 (18) | O12—C38—C33 | 109.01 (18) |
| C14—C9—C10 | 102.78 (19) | C37—C38—C33 | 102.50 (17) |
| O3—C9—C8 | 112.8 (2) | O12—C38—H38 | 108.8 |
| C14—C9—C8 | 109.8 (2) | C37—C38—H38 | 108.8 |
| C10—C9—C8 | 111.68 (17) | C33—C38—H38 | 108.8 |
| C9—C10—C12 | 103.03 (19) | C40—C39—C32 | 118.16 (18) |
| C9—C10—C11 | 117.51 (18) | C40—C39—H39A | 107.8 |
| C12—C10—C11 | 115.81 (19) | C32—C39—H39A | 107.8 |
| C9—C10—H10 | 106.6 | C40—C39—H39B | 107.8 |
| C12—C10—H10 | 106.6 | C32—C39—H39B | 107.8 |

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| C11—C10—H10 | 106.6 | H39A—C39—H39B | 107.1 |
| C17—C11—C1 | 116.23 (18) | O13—C40—C39 | 110.64 (18) |
| C17—C11—C5 | 98.06 (18) | O13—C40—C37 | 108.11 (18) |
| C1—C11—C5 | 112.57 (18) | C39—C40—C37 | 113.07 (19) |
| C17—C11—C10 | 109.21 (17) | O13—C40—H40 | 108.3 |
| C1—C11—C10 | 108.58 (18) | C39—C40—H40 | 108.3 |
| C5—C11—C10 | 111.92 (18) | C37—C40—H40 | 108.3 |
| C13—C12—C10 | 106.9 (2) | N4—C41—C35 | 108.80 (16) |
| C13—C12—H12A | 110.3 | N4—C41—C31 | 115.46 (16) |
| C10—C12—H12A | 110.3 | C35—C41—C31 | 100.84 (16) |
| C13—C12—H12B | 110.3 | N4—C41—H41 | 110.4 |
| C10—C12—H12B | 110.3 | C35—C41—H41 | 110.4 |
| H12A—C12—H12B | 108.6 | C31—C41—H41 | 110.4 |
| C14—C13—C16 | 112.5 (2) | N4—C42—C28 | 113.15 (17) |
| C14—C13—C12 | 99.8 (2) | N4—C42—H42A | 108.9 |
| C16—C13—C12 | 111.2 (2) | C28—C42—H42A | 108.9 |
| C14—C13—H13 | 111.0 | N4—C42—H42B | 108.9 |
| C16—C13—H13 | 111.0 | C28—C42—H42B | 108.9 |
| C12—C13—H13 | 111.0 | H42A—C42—H42B | 107.8 |
| O5—C14—C9 | 108.6 (2) | O8—C43—O9 | 122.2 (2) |
| O5—C14—C13 | 117.9 (2) | O8—C43—C1'' | 125.3 (2) |
| C9—C14—C13 | 102.86 (19) | O9—C43—C1'' | 112.53 (19) |
| O5—C14—H14 | 109.0 | O10—C44—H44A | 109.5 |
| C9—C14—H14 | 109.0 | O10—C44—H44B | 109.5 |
| C13—C14—H14 | 109.0 | H44A—C44—H44B | 109.5 |
| C16—C15—C8 | 119.1 (2) | O10—C44—H44C | 109.5 |
| C16—C15—H15A | 107.5 | H44A—C44—H44C | 109.5 |
| C8—C15—H15A | 107.5 | H44B—C44—H44C | 109.5 |
| C16—C15—H15B | 107.5 | O12—C45—H45A | 109.5 |
| C8—C15—H15B | 107.5 | O12—C45—H45B | 109.5 |
| H15A—C15—H15B | 107.0 | H45A—C45—H45B | 109.5 |
| O6—C16—C15 | 111.0 (2) | O12—C45—H45C | 109.5 |
| O6—C16—C13 | 107.2 (2) | H45A—C45—H45C | 109.5 |
| C15—C16—C13 | 113.5 (2) | H45B—C45—H45C | 109.5 |
| O6—C16—H16 | 108.3 | O13—C46—H46A | 109.5 |
| C15—C16—H16 | 108.3 | O13—C46—H46B | 109.5 |
| C13—C16—H16 | 108.3 | H46A—C46—H46B | 109.5 |
| N2—C17—C11 | 108.60 (17) | O13—C46—H46C | 109.5 |
| N2—C17—C7 | 115.47 (18) | H46A—C46—H46C | 109.5 |
| C11—C17—C7 | 100.71 (17) | H46B—C46—H46C | 109.5 |
| N2—C17—H17 | 110.5 | N4—C47—C48 | 114.3 (2) |
| C11—C17—H17 | 110.5 | N4—C47—H47A | 108.7 |
| C7—C17—H17 | 110.5 | C48—C47—H47A | 108.7 |
| N2—C18—C4 | 112.4 (2) | N4—C47—H47B | 108.7 |
| N2—C18—H18A | 109.1 | C48—C47—H47B | 108.7 |
| C4—C18—H18A | 109.1 | H47A—C47—H47B | 107.6 |
| N2—C18—H18B | 109.1 | C47—C48—H48A | 109.5 |
| C4—C18—H18B | 109.1 | C47—C48—H48B | 109.5 |

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| H18A—C18—H18B | 107.8 | H48A—C48—H48B | 109.5 |
| O1—C19—O2 | 123.0 (3) | C47—C48—H48C | 109.5 |
| O1—C19—C1' | 125.6 (3) | H48A—C48—H48C | 109.5 |
| O2—C19—C1' | 111.4 (2) | H48B—C48—H48C | 109.5 |
| O7—C20—H20A | 109.5 | C6'—C1'—C2' | 118.2 (3) |
| O7—C20—H20B | 109.5 | C6'—C1'—C19 | 119.7 (3) |
| H20A—C20—H20B | 109.5 | C2'—C1'—C19 | 122.0 (3) |
| O7—C20—H20C | 109.5 | N1—C2'—C3' | 119.0 (3) |
| H20A—C20—H20C | 109.5 | N1—C2'—C1' | 122.4 (3) |
| H20B—C20—H20C | 109.5 | C3'—C2'—C1' | 118.6 (3) |
| O6—C21—H21A | 109.5 | C4'—C3'—C2' | 121.3 (3) |
| O6—C21—H21B | 109.5 | C4'—C3'—H3' | 119.3 |
| H21A—C21—H21B | 109.5 | C2'—C3'—H3' | 119.3 |
| O6—C21—H21C | 109.5 | C3'—C4'—C5' | 120.0 (4) |
| H21A—C21—H21C | 109.5 | C3'—C4'—H4' | 120.0 |
| H21B—C21—H21C | 109.5 | C5'—C4'—H4' | 120.0 |
| O5—C22—H22A | 109.5 | C6'—C5'—C4' | 120.1 (4) |
| O5—C22—H22B | 109.5 | C6'—C5'—H5' | 120.0 |
| H22A—C22—H22B | 109.5 | C4'—C5'—H5' | 120.0 |
| O5—C22—H22C | 109.5 | C5'—C6'—C1' | 121.7 (3) |
| H22A—C22—H22C | 109.5 | C5'—C6'—H6' | 119.1 |
| H22B—C22—H22C | 109.5 | C1'—C6'—H6' | 119.1 |
| N2—C23—C24 | 113.5 (2) | C6''—C1''—C2'' | 118.3 (2) |
| N2—C23—H23A | 108.9 | C6''—C1''—C43 | 120.7 (2) |
| C24—C23—H23A | 108.9 | C2''—C1''—C43 | 120.9 (2) |
| N2—C23—H23B | 108.9 | N3—C2''—C3'' | 119.9 (3) |
| C24—C23—H23B | 108.9 | N3—C2''—C1'' | 122.0 (3) |
| H23A—C23—H23B | 107.7 | C3''—C2''—C1'' | 118.1 (3) |
| C23—C24—H24A | 109.5 | C4''—C3''—C2'' | 121.7 (3) |
| C23—C24—H24B | 109.5 | C4''—C3''—H3'' | 119.2 |
| H24A—C24—H24B | 109.5 | C2''—C3''—H3'' | 119.2 |
| C23—C24—H24C | 109.5 | C3''—C4''—C5'' | 120.1 (3) |
| H24A—C24—H24C | 109.5 | C3''—C4''—H4'' | 120.0 |
| H24B—C24—H24C | 109.5 | C5''—C4''—H4'' | 120.0 |
| O10—C25—C26 | 108.00 (17) | C6''—C5''—C4'' | 119.7 (3) |
| O10—C25—C35 | 109.78 (16) | C6''—C5''—H5'' | 120.1 |
| C26—C25—C35 | 116.81 (17) | C4''—C5''—H5'' | 120.1 |
| O10—C25—H25 | 107.3 | C5''—C6''—C1'' | 122.1 (2) |
| C26—C25—H25 | 107.3 | C5''—C6''—H6'' | 119.0 |
| C35—C25—H25 | 107.3 | C1''—C6''—H6'' | 119.0 |
| C27—C26—C25 | 113.19 (19) | C2'—N1—H1A | 108.9 |
| C27—C26—H26A | 108.9 | C2'—N1—H1B | 109.3 |
| C25—C26—H26A | 108.9 | H1A—N1—H1B | 109.5 |
| C27—C26—H26B | 108.9 | C23—N2—C18 | 111.77 (19) |
| C25—C26—H26B | 108.9 | C23—N2—C17 | 114.02 (19) |
| H26A—C26—H26B | 107.8 | C18—N2—C17 | 116.80 (18) |
| C26—C27—C28 | 109.07 (18) | C2''—N3—H3C | 108.5 |
| C26—C27—H27A | 109.9 | C2''—N3—H3D | 109.0 |

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| C28—C27—H27A | 109.9 | H3C—N3—H3D | 109.5 |
| C26—C27—H27B | 109.9 | C47—N4—C42 | 109.67 (17) |
| C28—C27—H27B | 109.9 | C47—N4—C41 | 114.24 (17) |
| H27A—C27—H27B | 108.3 | C42—N4—C41 | 117.19 (17) |
| O9—C28—C27 | 109.62 (17) | C19—O2—C4 | 124.4 (2) |
| O9—C28—C29 | 102.89 (16) | C9—O3—H3 | 109.5 |
| C27—C28—C29 | 110.14 (18) | C8—O4—H4 | 109.5 |
| O9—C28—C42 | 110.62 (17) | C22—O5—C14 | 113.9 (2) |
| C27—C28—C42 | 114.03 (18) | C21—O6—C16 | 112.6 (2) |
| C29—C28—C42 | 108.97 (17) | C20—O7—C1 | 114.2 (2) |
| C28—C29—C30 | 108.75 (17) | C43—O9—C28 | 122.13 (17) |
| C28—C29—C35 | 109.14 (17) | C25—O10—C44 | 113.1 (2) |
| C30—C29—C35 | 104.76 (17) | C32—O11—H11 | 109.4 |
| C28—C29—H29 | 111.3 | C45—O12—C38 | 112.77 (19) |
| C30—C29—H29 | 111.3 | C46—O13—C40 | 112.65 (18) |
| C35—C29—H29 | 111.3 | C33—O14—H14A | 109.3 |
| O7—C1—C2—C3 | 161.3 (2) | O14—C33—C34—C35 | -89.7 (2) |
| C11—C1—C2—C3 | 38.9 (3) | C38—C33—C34—C35 | 152.49 (18) |
| C1—C2—C3—C4 | -51.2 (3) | C32—C33—C34—C35 | 35.2 (3) |
| C2—C3—C4—O2 | 177.0 (2) | C28—C29—C35—C41 | -74.90 (19) |
| C2—C3—C4—C5 | 65.4 (3) | C30—C29—C35—C41 | 41.42 (19) |
| C2—C3—C4—C18 | -58.2 (3) | C28—C29—C35—C25 | 47.8 (2) |
| O2—C4—C5—C6 | 65.3 (2) | C30—C29—C35—C25 | 164.15 (17) |
| C3—C4—C5—C6 | -178.0 (2) | C28—C29—C35—C34 | 169.64 (16) |
| C18—C4—C5—C6 | -51.3 (2) | C30—C29—C35—C34 | -74.0 (2) |
| O2—C4—C5—C11 | 179.17 (18) | O10—C25—C35—C41 | -48.4 (2) |
| C3—C4—C5—C11 | -64.2 (3) | C26—C25—C35—C41 | 74.9 (2) |
| C18—C4—C5—C11 | 62.5 (2) | O10—C25—C35—C29 | -160.53 (17) |
| C4—C5—C6—C7 | 101.3 (2) | C26—C25—C35—C29 | -37.2 (3) |
| C11—C5—C6—C7 | -14.9 (2) | O10—C25—C35—C34 | 76.1 (2) |
| C5—C6—C7—C8 | 102.43 (19) | C26—C25—C35—C34 | -160.53 (19) |
| C5—C6—C7—C17 | -17.6 (2) | C33—C34—C35—C41 | -49.7 (2) |
| C6—C7—C8—O4 | 64.9 (2) | C36—C34—C35—C41 | 73.5 (2) |
| C17—C7—C8—O4 | 179.98 (18) | C33—C34—C35—C29 | 58.0 (2) |
| C6—C7—C8—C15 | -177.73 (19) | C36—C34—C35—C29 | -178.83 (17) |
| C17—C7—C8—C15 | -62.6 (2) | C33—C34—C35—C25 | -177.63 (18) |
| C6—C7—C8—C9 | -51.6 (2) | C36—C34—C35—C25 | -54.4 (2) |
| C17—C7—C8—C9 | 63.5 (2) | C33—C34—C36—C37 | 7.3 (2) |
| O4—C8—C9—O3 | -31.9 (2) | C35—C34—C36—C37 | -123.20 (19) |
| C7—C8—C9—O3 | 82.8 (2) | C34—C36—C37—C38 | -34.7 (2) |
| C15—C8—C9—O3 | -151.70 (19) | C34—C36—C37—C40 | 84.5 (2) |
| O4—C8—C9—C14 | 91.7 (2) | C40—C37—C38—O12 | 52.1 (3) |
| C7—C8—C9—C14 | -153.64 (19) | C36—C37—C38—O12 | 169.60 (18) |
| C15—C8—C9—C14 | -28.1 (3) | C40—C37—C38—C33 | -68.0 (2) |
| O4—C8—C9—C10 | -155.01 (18) | C36—C37—C38—C33 | 49.5 (2) |
| C7—C8—C9—C10 | -40.3 (3) | O14—C33—C38—O12 | 71.7 (2) |
| C15—C8—C9—C10 | 85.2 (2) | C34—C33—C38—O12 | -172.71 (17) |

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| O3—C9—C10—C12 | 143.00 (19) | C32—C33—C38—O12 | -54.1 (2) |
| C14—C9—C10—C12 | 25.9 (2) | O14—C33—C38—C37 | -161.82 (18) |
| C8—C9—C10—C12 | -91.8 (2) | C34—C33—C38—C37 | -46.2 (2) |
| O3—C9—C10—C11 | -88.4 (2) | C32—C33—C38—C37 | 72.4 (2) |
| C14—C9—C10—C11 | 154.5 (2) | O11—C32—C39—C40 | -143.67 (19) |
| C8—C9—C10—C11 | 36.9 (3) | C31—C32—C39—C40 | 101.0 (2) |
| O7—C1—C11—C17 | -47.8 (3) | C33—C32—C39—C40 | -23.9 (3) |
| C2—C1—C11—C17 | 74.3 (3) | C32—C39—C40—O13 | 150.93 (19) |
| O7—C1—C11—C5 | -159.75 (19) | C32—C39—C40—C37 | 29.5 (3) |
| C2—C1—C11—C5 | -37.6 (3) | C38—C37—C40—O13 | -105.1 (2) |
| O7—C1—C11—C10 | 75.8 (2) | C36—C37—C40—O13 | 144.42 (19) |
| C2—C1—C11—C10 | -162.1 (2) | C38—C37—C40—C39 | 17.8 (3) |
| C4—C5—C11—C17 | -74.4 (2) | C36—C37—C40—C39 | -92.7 (2) |
| C6—C5—C11—C17 | 41.2 (2) | C29—C35—C41—N4 | 69.81 (19) |
| C4—C5—C11—C1 | 48.4 (2) | C25—C35—C41—N4 | -50.6 (2) |
| C6—C5—C11—C1 | 164.07 (18) | C34—C35—C41—N4 | -174.11 (16) |
| C4—C5—C11—C10 | 171.08 (18) | C29—C35—C41—C31 | -52.03 (17) |
| C6—C5—C11—C10 | -73.3 (2) | C25—C35—C41—C31 | -172.41 (16) |
| C9—C10—C11—C17 | -51.6 (3) | C34—C35—C41—C31 | 64.05 (19) |
| C12—C10—C11—C17 | 70.7 (3) | C30—C31—C41—N4 | -73.1 (2) |
| C9—C10—C11—C1 | -179.26 (19) | C32—C31—C41—N4 | 167.96 (17) |
| C12—C10—C11—C1 | -57.0 (3) | C30—C31—C41—C35 | 43.99 (19) |
| C9—C10—C11—C5 | 55.9 (3) | C32—C31—C41—C35 | -75.0 (2) |
| C12—C10—C11—C5 | 178.2 (2) | O9—C28—C42—N4 | -153.09 (17) |
| C9—C10—C12—C13 | 3.5 (2) | C27—C28—C42—N4 | 82.8 (2) |
| C11—C10—C12—C13 | -126.2 (2) | C29—C28—C42—N4 | -40.7 (2) |
| C10—C12—C13—C14 | -31.2 (3) | O1—C19—C1'—C6' | 179.2 (3) |
| C10—C12—C13—C16 | 87.7 (3) | O2—C19—C1'—C6' | -0.1 (4) |
| O3—C9—C14—O5 | 71.1 (2) | O1—C19—C1'—C2' | 3.2 (5) |
| C10—C9—C14—O5 | -172.86 (18) | O2—C19—C1'—C2' | -176.2 (3) |
| C8—C9—C14—O5 | -53.9 (3) | C6'—C1'—C2'—N1 | 179.3 (3) |
| O3—C9—C14—C13 | -163.2 (2) | C19—C1'—C2'—N1 | -4.6 (5) |
| C10—C9—C14—C13 | -47.2 (2) | C6'—C1'—C2'—C3' | -1.6 (4) |
| C8—C9—C14—C13 | 71.8 (2) | C19—C1'—C2'—C3' | 174.5 (3) |
| C16—C13—C14—O5 | 49.6 (3) | N1—C2'—C3'—C4' | -179.0 (4) |
| C12—C13—C14—O5 | 167.5 (2) | C1'—C2'—C3'—C4' | 1.9 (5) |
| C16—C13—C14—C9 | -69.9 (3) | C2'—C3'—C4'—C5' | -0.3 (7) |
| C12—C13—C14—C9 | 48.1 (2) | C3'—C4'—C5'—C6' | -1.4 (8) |
| O4—C8—C15—C16 | -140.2 (2) | C4'—C5'—C6'—C1' | 1.6 (8) |
| C7—C8—C15—C16 | 104.0 (2) | C2'—C1'—C6'—C5' | -0.1 (6) |
| C9—C8—C15—C16 | -20.4 (3) | C19—C1'—C6'—C5' | -176.3 (4) |
| C8—C15—C16—O6 | 144.3 (2) | O8—C43—C1''—C6'' | 174.7 (2) |
| C8—C15—C16—C13 | 23.5 (3) | O9—C43—C1''—C6'' | -4.4 (3) |
| C14—C13—C16—O6 | -100.5 (3) | O8—C43—C1''—C2'' | -3.5 (4) |
| C12—C13—C16—O6 | 148.5 (2) | O9—C43—C1''—C2'' | 177.4 (2) |
| C14—C13—C16—C15 | 22.4 (3) | C6''—C1''—C2''—N3 | 178.6 (3) |
| C12—C13—C16—C15 | -88.6 (3) | C43—C1''—C2''—N3 | -3.1 (4) |
| C1—C11—C17—N2 | -50.0 (3) | C6''—C1''—C2''—C3'' | 0.6 (4) |

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| C5—C11—C17—N2 | 70.1 (2) | C43—C1"—C2"—C3" | 178.9 (3) |
| C10—C11—C17—N2 | -173.27 (17) | N3—C2"—C3"—C4" | -179.6 (3) |
| C1—C11—C17—C7 | -171.74 (19) | C1"—C2"—C3"—C4" | -1.6 (5) |
| C5—C11—C17—C7 | -51.62 (19) | C2"—C3"—C4"—C5" | 1.8 (5) |
| C10—C11—C17—C7 | 65.0 (2) | C3"—C4"—C5"—C6" | -1.1 (5) |
| C8—C7—C17—N2 | 167.96 (18) | C4"—C5"—C6"—C1" | 0.2 (4) |
| C6—C7—C17—N2 | -72.8 (2) | C2"—C1"—C6"—C5" | 0.0 (4) |
| C8—C7—C17—C11 | -75.3 (2) | C43—C1"—C6"—C5" | -178.3 (2) |
| C6—C7—C17—C11 | 44.0 (2) | C24—C23—N2—C18 | 157.0 (2) |
| O2—C4—C18—N2 | -153.59 (18) | C24—C23—N2—C17 | -67.8 (3) |
| C3—C4—C18—N2 | 82.0 (3) | C4—C18—N2—C23 | 176.49 (19) |
| C5—C4—C18—N2 | -42.6 (3) | C4—C18—N2—C17 | 42.6 (3) |
| O10—C25—C26—C27 | 164.22 (19) | C11—C17—N2—C23 | 168.01 (19) |
| C35—C25—C26—C27 | 40.0 (3) | C7—C17—N2—C23 | -79.8 (3) |
| C25—C26—C27—C28 | -53.2 (3) | C11—C17—N2—C18 | -59.1 (2) |
| C26—C27—C28—O9 | 179.43 (18) | C7—C17—N2—C18 | 53.0 (3) |
| C26—C27—C28—C29 | 66.9 (2) | C48—C47—N4—C42 | 165.8 (2) |
| C26—C27—C28—C42 | -55.9 (3) | C48—C47—N4—C41 | -60.4 (3) |
| O9—C28—C29—C30 | 65.5 (2) | C28—C42—N4—C47 | 172.51 (19) |
| C27—C28—C29—C30 | -177.69 (18) | C28—C42—N4—C41 | 40.2 (2) |
| C42—C28—C29—C30 | -51.9 (2) | C35—C41—N4—C47 | 172.30 (19) |
| O9—C28—C29—C35 | 179.26 (16) | C31—C41—N4—C47 | -75.2 (2) |
| C27—C28—C29—C35 | -63.9 (2) | C35—C41—N4—C42 | -57.4 (2) |
| C42—C28—C29—C35 | 61.8 (2) | C31—C41—N4—C42 | 55.0 (2) |
| C28—C29—C30—C31 | 101.63 (19) | O1—C19—O2—C4 | -7.9 (4) |
| C35—C29—C30—C31 | -15.0 (2) | C1'—C19—O2—C4 | 171.5 (2) |
| C29—C30—C31—C32 | 101.46 (19) | C3—C4—O2—C19 | 73.0 (3) |
| C29—C30—C31—C41 | -17.4 (2) | C5—C4—O2—C19 | -169.6 (2) |
| C30—C31—C32—O11 | 67.1 (2) | C18—C4—O2—C19 | -54.0 (3) |
| C41—C31—C32—O11 | -179.00 (17) | C9—C14—O5—C22 | -160.9 (3) |
| C30—C31—C32—C39 | -175.93 (17) | C13—C14—O5—C22 | 82.7 (3) |
| C41—C31—C32—C39 | -62.0 (2) | C15—C16—O6—C21 | 68.2 (4) |
| C30—C31—C32—C33 | -49.7 (2) | C13—C16—O6—C21 | -167.3 (3) |
| C41—C31—C32—C33 | 64.3 (2) | C2—C1—O7—C20 | 81.8 (3) |
| O11—C32—C33—O14 | -33.1 (2) | C11—C1—O7—C20 | -150.6 (3) |
| C31—C32—C33—O14 | 81.5 (2) | O8—C43—O9—C28 | 3.2 (3) |
| C39—C32—C33—O14 | -152.54 (18) | C1"—C43—O9—C28 | -177.64 (18) |
| O11—C32—C33—C38 | 91.7 (2) | C27—C28—O9—C43 | 70.0 (2) |
| C31—C32—C33—C38 | -153.70 (18) | C29—C28—O9—C43 | -172.83 (18) |
| C39—C32—C33—C38 | -27.8 (2) | C42—C28—O9—C43 | -56.6 (2) |
| O11—C32—C33—C34 | -155.17 (17) | C26—C25—O10—C44 | 79.8 (2) |
| C31—C32—C33—C34 | -40.6 (2) | C35—C25—O10—C44 | -151.8 (2) |
| C39—C32—C33—C34 | 85.4 (2) | C37—C38—O12—C45 | 64.2 (3) |
| O14—C33—C34—C36 | 140.79 (18) | C33—C38—O12—C45 | -179.2 (2) |
| C38—C33—C34—C36 | 22.9 (2) | C39—C40—O13—C46 | 75.9 (3) |
| C32—C33—C34—C36 | -94.3 (2) | C37—C40—O13—C46 | -159.8 (2) |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| O14—H14A \cdots O6 ⁱ | 0.98 | 2.27 | 2.927 (2) | 123 |
| O11—H11 \cdots O12 | 0.84 | 2.40 | 2.944 (2) | 124 |
| O4—H4 \cdots O5 | 0.84 | 2.33 | 2.914 (3) | 127 |
| O3—H3 \cdots O13 ⁱⁱ | 0.84 | 2.41 | 3.095 (2) | 139 |
| N3—H3D \cdots O8 | 0.91 | 2.02 | 2.687 (3) | 129 |
| N1—H1A \cdots O1 | 0.91 | 2.02 | 2.752 (4) | 137 |

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