



Crystal structure of 14-methyl-11-(3-methylphenyl)-12-oxa-8,14-diazatetracyclo[8.3.3.0^{1,10}.0^{2,7}]hexadeca-2(7),3,5-triene-9,13-dione

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Received 28 January 2015; accepted 23 April 2015

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

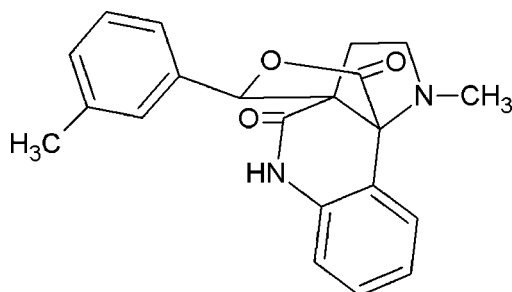
In the title compound, C₂₁H₂₀N₂O₃, the lactone ring adopts an envelope conformation with the quaternary C atom bonded to two other C atoms as the flap. The fused pyrrolidine ring adopts a twisted conformation about the C_q—N (q = quaternary) bond. In the crystal, inversion dimers linked by pairs of N—H...O hydrogen bonds generate R₂²(8) loops. The dimers are linked into [110] chains by pairs of C—H...O interactions, which generate R₂²(14) loops.

Keywords: crystal structure; tetracyclo; hexadecatrienedione; hydrogen bonding.

CCDC reference: 1061495

1. Related literature

For related structures, see: Ramesh *et al.* (2008); Zhao & Teng (2008); Bai *et al.* (2009); Du *et al.* (2010); Wang *et al.* (2010). For puckering parameters, see: Cremer & Pople (1975).



2. Experimental

2.1. Crystal data

| | |
|---|---|
| C ₂₁ H ₂₀ N ₂ O ₃ | $V = 1737.2 (2) \text{ \AA}^3$ |
| $M_r = 348.39$ | $Z = 4$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 10.4772 (7) \text{ \AA}$ | $\mu = 0.09 \text{ mm}^{-1}$ |
| $b = 8.6834 (6) \text{ \AA}$ | $T = 293 \text{ K}$ |
| $c = 19.1123 (13) \text{ \AA}$ | $0.35 \times 0.30 \times 0.30 \text{ mm}$ |
| $\beta = 92.490 (2)^\circ$ | |

2.2. Data collection

| | |
|--|--|
| Bruker Kappa APEXII CCD diffractometer | 25650 measured reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2004) | 3787 independent reflections |
| $T_{\min} = 0.969$, $T_{\max} = 0.974$ | 2875 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.024$ |

2.3. Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.045$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.137$ | $\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$ |
| $S = 1.09$ | $\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$ |
| 3787 reflections | |
| 239 parameters | |

Table 1

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|----------|-------------|-------------|---------------|
| $\text{N2}-\text{H2A}\cdots\text{O3}^i$ | 0.91 (2) | 1.93 (2) | 2.802 (2) | 159.6 (19) |
| $\text{C5}-\text{H5}\cdots\text{O2}^{ii}$ | 0.93 | 2.55 | 3.303 (3) | 138 |

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2009).

Acknowledgements

MPS and ASP thank Dr Babu Vargheese, SAIF, IIT, Madras, India, for the data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7360).

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supporting information

Acta Cryst. (2015). E71, o379–o380 [doi:10.1107/S2056989015008129]

Crystal structure of 14-methyl-11-(3-methylphenyl)-12-oxa-8,14-diazatetracyclo[8.3.3.0^{1,10}.0^{2,7}]hexadeca-2(7),3,5-triene-9,13-dione

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S1. Comment

The geometric parameters of the title molecule (Fig. 1) agree well with reported similar structures (Ramesh *et al.*, 2008; Zhao & Teng, 2008; Bai *et al.*, 2009; Du *et al.*, 2010; Wang *et al.*, 2010). The five-membered furan ring (atoms O1/C7–C10) adopts an envelope conformation, with atom C10 as the flap, with puckering parameters (Cremer & Pople, 1975), $q_2 = 0.4062(2)$ Å and $\varphi_2 = 246.5(2)^\circ$ and the pyrrolidine ring (atoms N1/C9–C12) exhibits a twisted conformation as indicated by the puckering parameters $q_2 = 0.3981(2)$ Å and $\varphi_2 = 22.4(3)^\circ$. The quinoline ring system is roughly planar, with a maximum deviation of $0.315(2)$ Å for atom C10 and the plane of the furan ring is oriented at dihedral angles of $72.5(8)$ and $77.9(1)^\circ$ with respect to the quinoline and pyrrolidine rings, respectively.

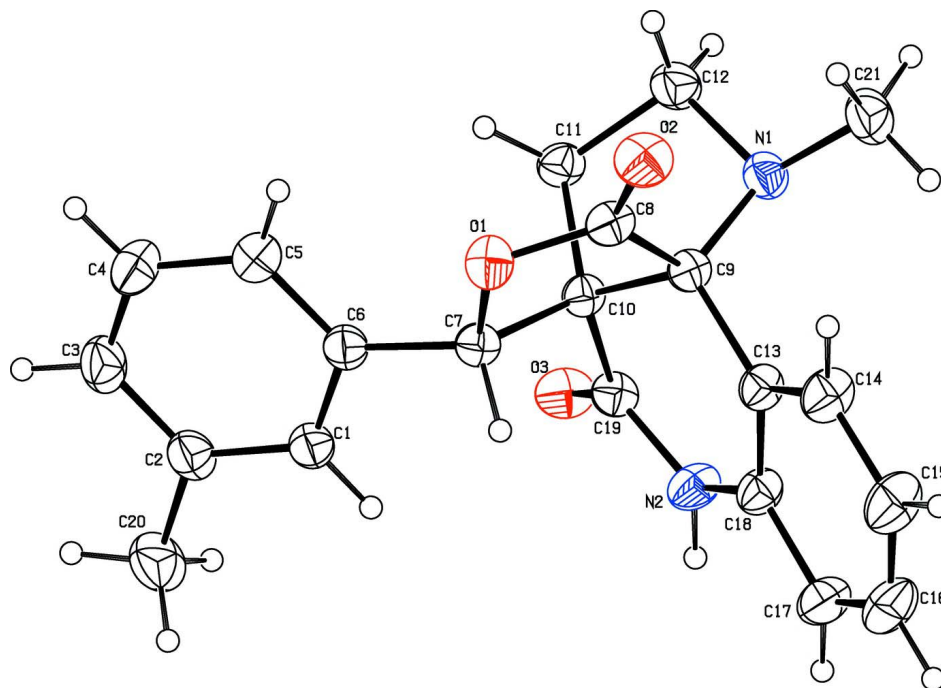
In the crystal, hydrogen-bonded chains running along [110] are generated by connecting neighbouring molecules *via* C—H \cdots O and N—H \cdots O hydrogen bonds, forming a chain. Intermolecular C5—H5 \cdots O2 hydrogen bonding forms an $R_2^2(14)$ graph-set dimer (Fig. 2 and Table 1). In addition to this, another graph-set dimer of $R_2^2(8)$ forms in the unit cell involving N2—H2A \cdots O3 hydrogen bonds (Fig. 2).

S2. Experimental

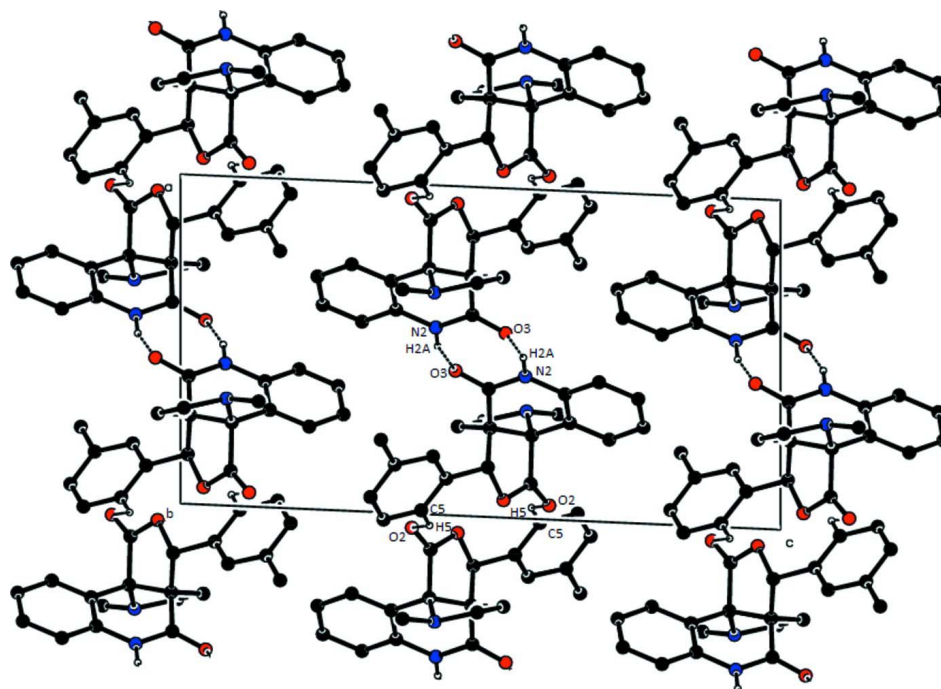
A mixture of methyl 2-(hydroxy(m-tolyl)methyl)acrylate (1 mmol), isatin (1.1 mmol) and sarcosine (1.1 mmol) was placed in a round bottom flask and melted at 180°C until completion of the reaction was evidenced by TLC analysis. After completion of the reaction, the crude product was washed with 5ml of ethylacetate and hexane mixture (1:4 ratio) which successfully provided the pure product as colorless solid. The product was dissolved in ethyl acetate and heated for two minutes. The resulting solution was subjected to crystallization by slow evaporation of the solvent for 48 hours resulting in the formation of colourless blocks.

S3. Refinement

All H atoms were fixed geometrically and allowed to ride on their parent C atoms, with C-H distances fixed in the range $0.93\text{--}0.98$ Å with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H $1.2U_{\text{eq}}(\text{C})$ for other H atoms.

**Figure 1**

The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level.

**Figure 2**

The molecular packing is viewed along the *b* axis. Dashed lines show the intermolecular C-H...O and N-H...O hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted for clarity.

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Hall symbol: -P 2ybc

 $a = 10.4772$ (7) Å $b = 8.6834$ (6) Å $c = 19.1123$ (13) Å $\beta = 92.490$ (2)° $V = 1737.2$ (2) Å³ $Z = 4$ $F(000) = 736$ $D_x = 1.332$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3787 reflections

 $\theta = 2.1$ – 27.0 ° $\mu = 0.09$ mm⁻¹ $T = 293$ K

Block, colourless

 $0.35 \times 0.30 \times 0.30$ mm*Data collection*

Bruker Kappa APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 ω and φ scans

Absorption correction: multi-scan

(SADABS; Bruker, 2004)

 $T_{\min} = 0.969$, $T_{\max} = 0.974$

25650 measured reflections

3787 independent reflections

2875 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.024$ $\theta_{\text{max}} = 27.0$ °, $\theta_{\text{min}} = 2.1$ ° $h = -13$ → 13 $k = -11$ → 11 $l = -24$ → 24 *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.045$ $wR(F^2) = 0.137$ $S = 1.09$

3787 reflections

239 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 atoms treated by a mixture of independent and constrained refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 0.7606P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.29$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³*Special details*

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|--------------|--------------|-------------|----------------------------------|
| O1 | 0.05279 (11) | 0.22692 (16) | 0.53826 (6) | 0.0458 (3) |
| O3 | 0.43975 (13) | 0.34579 (16) | 0.45820 (6) | 0.0505 (4) |
| O2 | 0.04279 (13) | 0.03341 (17) | 0.61440 (7) | 0.0557 (4) |

| | | | | |
|------|--------------|---------------|--------------|------------|
| N1 | 0.32532 (15) | -0.00285 (17) | 0.57673 (7) | 0.0427 (4) |
| N2 | 0.43155 (15) | 0.38257 (19) | 0.57461 (8) | 0.0454 (4) |
| C9 | 0.25355 (16) | 0.13927 (19) | 0.58542 (8) | 0.0342 (4) |
| C7 | 0.15071 (16) | 0.32733 (19) | 0.51218 (8) | 0.0368 (4) |
| H7 | 0.1649 | 0.4112 | 0.5459 | 0.044* |
| C10 | 0.27021 (15) | 0.22222 (19) | 0.51571 (8) | 0.0334 (4) |
| C13 | 0.29625 (17) | 0.2330 (2) | 0.64871 (8) | 0.0381 (4) |
| C19 | 0.38880 (16) | 0.3193 (2) | 0.51367 (8) | 0.0378 (4) |
| C18 | 0.38303 (17) | 0.3521 (2) | 0.64055 (9) | 0.0404 (4) |
| C11 | 0.27058 (18) | 0.0894 (2) | 0.46208 (9) | 0.0401 (4) |
| H11A | 0.1898 | 0.0847 | 0.4353 | 0.048* |
| H11B | 0.3389 | 0.1028 | 0.4300 | 0.048* |
| C14 | 0.2508 (2) | 0.2060 (3) | 0.71465 (9) | 0.0522 (5) |
| H14 | 0.1914 | 0.1280 | 0.7206 | 0.063* |
| C6 | 0.11100 (17) | 0.3972 (2) | 0.44276 (9) | 0.0400 (4) |
| C1 | 0.17662 (19) | 0.5259 (2) | 0.42071 (9) | 0.0436 (4) |
| H1 | 0.2427 | 0.5654 | 0.4494 | 0.052* |
| C8 | 0.10628 (17) | 0.1232 (2) | 0.58346 (9) | 0.0403 (4) |
| C12 | 0.2914 (2) | -0.0568 (2) | 0.50569 (10) | 0.0496 (5) |
| H12A | 0.2141 | -0.1184 | 0.5052 | 0.059* |
| H12B | 0.3598 | -0.1184 | 0.4876 | 0.059* |
| C2 | 0.1465 (2) | 0.5974 (2) | 0.35712 (9) | 0.0483 (5) |
| C17 | 0.4237 (2) | 0.4417 (2) | 0.69755 (10) | 0.0534 (5) |
| H17 | 0.4813 | 0.5217 | 0.6918 | 0.064* |
| C5 | 0.0112 (2) | 0.3400 (2) | 0.40112 (10) | 0.0530 (5) |
| H5 | -0.0334 | 0.2535 | 0.4150 | 0.064* |
| C3 | 0.0451 (2) | 0.5388 (3) | 0.31651 (10) | 0.0568 (5) |
| H3 | 0.0221 | 0.5854 | 0.2740 | 0.068* |
| C16 | 0.3779 (2) | 0.4109 (3) | 0.76275 (10) | 0.0624 (6) |
| H16 | 0.4051 | 0.4704 | 0.8010 | 0.075* |
| C20 | 0.2201 (3) | 0.7356 (3) | 0.33399 (12) | 0.0682 (6) |
| H20A | 0.1865 | 0.7692 | 0.2890 | 0.102* |
| H20B | 0.3085 | 0.7086 | 0.3307 | 0.102* |
| H20C | 0.2123 | 0.8171 | 0.3674 | 0.102* |
| C4 | -0.0220 (2) | 0.4130 (3) | 0.33825 (11) | 0.0627 (6) |
| H4 | -0.0905 | 0.3761 | 0.3105 | 0.075* |
| C15 | 0.2922 (2) | 0.2928 (3) | 0.77163 (10) | 0.0639 (6) |
| H15 | 0.2624 | 0.2719 | 0.8158 | 0.077* |
| C21 | 0.3205 (2) | -0.1220 (2) | 0.63015 (11) | 0.0571 (5) |
| H21A | 0.3721 | -0.2079 | 0.6171 | 0.086* |
| H21B | 0.2338 | -0.1553 | 0.6343 | 0.086* |
| H21C | 0.3524 | -0.0814 | 0.6742 | 0.086* |
| H2A | 0.488 (2) | 0.461 (3) | 0.5713 (11) | 0.058 (6)* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|------------|------------|------------|-------------|------------|------------|
| O1 | 0.0362 (6) | 0.0560 (8) | 0.0455 (7) | -0.0010 (6) | 0.0058 (5) | 0.0056 (6) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| O3 | 0.0578 (8) | 0.0531 (8) | 0.0422 (7) | -0.0136 (6) | 0.0208 (6) | -0.0003 (6) |
| O2 | 0.0497 (8) | 0.0598 (9) | 0.0586 (8) | -0.0169 (7) | 0.0140 (6) | 0.0077 (7) |
| N1 | 0.0495 (9) | 0.0392 (8) | 0.0393 (8) | 0.0024 (7) | 0.0011 (6) | 0.0039 (6) |
| N2 | 0.0459 (9) | 0.0520 (9) | 0.0384 (8) | -0.0206 (8) | 0.0050 (6) | 0.0006 (7) |
| C9 | 0.0368 (9) | 0.0367 (8) | 0.0294 (7) | -0.0049 (7) | 0.0052 (6) | 0.0018 (6) |
| C7 | 0.0386 (9) | 0.0372 (9) | 0.0350 (8) | -0.0003 (7) | 0.0050 (7) | -0.0011 (7) |
| C10 | 0.0368 (8) | 0.0365 (9) | 0.0273 (7) | -0.0028 (7) | 0.0051 (6) | -0.0004 (6) |
| C13 | 0.0397 (9) | 0.0444 (9) | 0.0306 (8) | -0.0034 (7) | 0.0040 (7) | 0.0009 (7) |
| C19 | 0.0403 (9) | 0.0380 (9) | 0.0356 (8) | -0.0039 (7) | 0.0085 (7) | 0.0025 (7) |
| C18 | 0.0421 (9) | 0.0465 (10) | 0.0326 (8) | -0.0052 (8) | 0.0014 (7) | -0.0011 (7) |
| C11 | 0.0482 (10) | 0.0398 (9) | 0.0325 (8) | -0.0019 (8) | 0.0048 (7) | -0.0033 (7) |
| C14 | 0.0586 (12) | 0.0651 (13) | 0.0335 (9) | -0.0121 (10) | 0.0087 (8) | 0.0021 (8) |
| C6 | 0.0464 (10) | 0.0385 (9) | 0.0349 (8) | 0.0074 (8) | 0.0008 (7) | -0.0044 (7) |
| C1 | 0.0537 (11) | 0.0389 (9) | 0.0378 (9) | 0.0048 (8) | -0.0012 (8) | -0.0021 (7) |
| C8 | 0.0418 (9) | 0.0436 (10) | 0.0360 (8) | -0.0073 (8) | 0.0067 (7) | -0.0022 (7) |
| C12 | 0.0635 (12) | 0.0413 (10) | 0.0439 (10) | 0.0054 (9) | 0.0022 (9) | -0.0039 (8) |
| C2 | 0.0645 (12) | 0.0422 (10) | 0.0385 (9) | 0.0111 (9) | 0.0053 (8) | -0.0008 (8) |
| C17 | 0.0569 (12) | 0.0552 (12) | 0.0475 (11) | -0.0128 (10) | -0.0047 (9) | -0.0069 (9) |
| C5 | 0.0566 (12) | 0.0515 (11) | 0.0500 (11) | -0.0028 (9) | -0.0066 (9) | -0.0009 (9) |
| C3 | 0.0751 (14) | 0.0579 (12) | 0.0368 (10) | 0.0158 (11) | -0.0030 (9) | 0.0020 (9) |
| C16 | 0.0726 (15) | 0.0767 (15) | 0.0374 (10) | -0.0030 (12) | -0.0059 (9) | -0.0158 (10) |
| C20 | 0.0925 (18) | 0.0582 (13) | 0.0540 (12) | 0.0012 (12) | 0.0053 (12) | 0.0138 (10) |
| C4 | 0.0667 (14) | 0.0691 (15) | 0.0507 (12) | 0.0009 (12) | -0.0169 (10) | -0.0063 (11) |
| C15 | 0.0738 (15) | 0.0882 (17) | 0.0303 (9) | -0.0080 (13) | 0.0075 (9) | -0.0051 (10) |
| C21 | 0.0636 (13) | 0.0513 (12) | 0.0559 (12) | 0.0000 (10) | -0.0032 (10) | 0.0159 (9) |

Geometric parameters (Å, °)

| | | | |
|---------|-------------|----------|-----------|
| O1—C8 | 1.353 (2) | C14—H14 | 0.9300 |
| O1—C7 | 1.451 (2) | C6—C5 | 1.378 (3) |
| O3—C19 | 1.2292 (19) | C6—C1 | 1.387 (3) |
| O2—C8 | 1.197 (2) | C1—C2 | 1.389 (2) |
| N1—C21 | 1.456 (2) | C1—H1 | 0.9300 |
| N1—C9 | 1.458 (2) | C12—H12A | 0.9700 |
| N1—C12 | 1.465 (2) | C12—H12B | 0.9700 |
| N2—C19 | 1.347 (2) | C2—C3 | 1.385 (3) |
| N2—C18 | 1.404 (2) | C2—C20 | 1.503 (3) |
| N2—H2A | 0.91 (2) | C17—C16 | 1.381 (3) |
| C9—C13 | 1.510 (2) | C17—H17 | 0.9300 |
| C9—C10 | 1.531 (2) | C5—C4 | 1.389 (3) |
| C9—C8 | 1.548 (2) | C5—H5 | 0.9300 |
| C7—C6 | 1.501 (2) | C3—C4 | 1.374 (3) |
| C7—C10 | 1.548 (2) | C3—H3 | 0.9300 |
| C7—H7 | 0.9800 | C16—C15 | 1.378 (3) |
| C10—C19 | 1.504 (2) | C16—H16 | 0.9300 |
| C10—C11 | 1.543 (2) | C20—H20A | 0.9600 |
| C13—C14 | 1.386 (2) | C20—H20B | 0.9600 |
| C13—C18 | 1.390 (2) | C20—H20C | 0.9600 |

| | | | |
|---------------|-------------|---------------|-------------|
| C18—C17 | 1.390 (2) | C4—H4 | 0.9300 |
| C11—C12 | 1.529 (3) | C15—H15 | 0.9300 |
| C11—H11A | 0.9700 | C21—H21A | 0.9600 |
| C11—H11B | 0.9700 | C21—H21B | 0.9600 |
| C14—C15 | 1.379 (3) | C21—H21C | 0.9600 |
| C8—O1—C7 | 109.89 (13) | C6—C1—C2 | 121.97 (18) |
| C21—N1—C9 | 119.19 (15) | C6—C1—H1 | 119.0 |
| C21—N1—C12 | 114.09 (16) | C2—C1—H1 | 119.0 |
| C9—N1—C12 | 105.69 (13) | O2—C8—O1 | 121.69 (17) |
| C19—N2—C18 | 125.42 (15) | O2—C8—C9 | 128.41 (17) |
| C19—N2—H2A | 116.1 (14) | O1—C8—C9 | 109.88 (14) |
| C18—N2—H2A | 117.9 (14) | N1—C12—C11 | 105.24 (14) |
| N1—C9—C13 | 114.29 (14) | N1—C12—H12A | 110.7 |
| N1—C9—C10 | 102.71 (12) | C11—C12—H12A | 110.7 |
| C13—C9—C10 | 113.74 (13) | N1—C12—H12B | 110.7 |
| N1—C9—C8 | 116.04 (14) | C11—C12—H12B | 110.7 |
| C13—C9—C8 | 109.18 (13) | H12A—C12—H12B | 108.8 |
| C10—C9—C8 | 99.93 (13) | C3—C2—C1 | 117.75 (19) |
| O1—C7—C6 | 111.93 (14) | C3—C2—C20 | 121.27 (18) |
| O1—C7—C10 | 102.31 (13) | C1—C2—C20 | 120.97 (19) |
| C6—C7—C10 | 117.98 (13) | C16—C17—C18 | 119.49 (19) |
| O1—C7—H7 | 108.1 | C16—C17—H17 | 120.3 |
| C6—C7—H7 | 108.1 | C18—C17—H17 | 120.3 |
| C10—C7—H7 | 108.1 | C6—C5—C4 | 119.4 (2) |
| C19—C10—C9 | 114.33 (13) | C6—C5—H5 | 120.3 |
| C19—C10—C11 | 112.09 (13) | C4—C5—H5 | 120.3 |
| C9—C10—C11 | 103.29 (13) | C4—C3—C2 | 120.85 (19) |
| C19—C10—C7 | 109.63 (14) | C4—C3—H3 | 119.6 |
| C9—C10—C7 | 101.11 (12) | C2—C3—H3 | 119.6 |
| C11—C10—C7 | 115.91 (14) | C15—C16—C17 | 120.59 (19) |
| C14—C13—C18 | 118.69 (16) | C15—C16—H16 | 119.7 |
| C14—C13—C9 | 122.39 (16) | C17—C16—H16 | 119.7 |
| C18—C13—C9 | 118.92 (14) | C2—C20—H20A | 109.5 |
| O3—C19—N2 | 121.95 (16) | C2—C20—H20B | 109.5 |
| O3—C19—C10 | 121.17 (15) | H20A—C20—H20B | 109.5 |
| N2—C19—C10 | 116.77 (14) | C2—C20—H20C | 109.5 |
| C13—C18—C17 | 120.52 (16) | H20A—C20—H20C | 109.5 |
| C13—C18—N2 | 120.33 (15) | H20B—C20—H20C | 109.5 |
| C17—C18—N2 | 119.15 (17) | C3—C4—C5 | 120.8 (2) |
| C12—C11—C10 | 105.24 (13) | C3—C4—H4 | 119.6 |
| C12—C11—H11A | 110.7 | C5—C4—H4 | 119.6 |
| C10—C11—H11A | 110.7 | C16—C15—C14 | 119.58 (19) |
| C12—C11—H11B | 110.7 | C16—C15—H15 | 120.2 |
| C10—C11—H11B | 110.7 | C14—C15—H15 | 120.2 |
| H11A—C11—H11B | 108.8 | N1—C21—H21A | 109.5 |
| C15—C14—C13 | 121.12 (19) | N1—C21—H21B | 109.5 |
| C15—C14—H14 | 119.4 | H21A—C21—H21B | 109.5 |

| | | | |
|-----------------|--------------|-----------------|--------------|
| C13—C14—H14 | 119.4 | N1—C21—H21C | 109.5 |
| C5—C6—C1 | 119.21 (17) | H21A—C21—H21C | 109.5 |
| C5—C6—C7 | 122.61 (17) | H21B—C21—H21C | 109.5 |
| C1—C6—C7 | 118.17 (16) | | |
| | | | |
| C21—N1—C9—C13 | 63.0 (2) | C14—C13—C18—N2 | 179.77 (18) |
| C12—N1—C9—C13 | -167.01 (14) | C9—C13—C18—N2 | -1.1 (3) |
| C21—N1—C9—C10 | -173.31 (15) | C19—N2—C18—C13 | 9.7 (3) |
| C12—N1—C9—C10 | -43.33 (17) | C19—N2—C18—C17 | -170.84 (18) |
| C21—N1—C9—C8 | -65.4 (2) | C19—C10—C11—C12 | 108.42 (17) |
| C12—N1—C9—C8 | 64.55 (18) | C9—C10—C11—C12 | -15.13 (18) |
| C8—O1—C7—C6 | 156.13 (14) | C7—C10—C11—C12 | -124.70 (16) |
| C8—O1—C7—C10 | 28.85 (16) | C18—C13—C14—C15 | -1.3 (3) |
| N1—C9—C10—C19 | -86.79 (16) | C9—C13—C14—C15 | 179.6 (2) |
| C13—C9—C10—C19 | 37.3 (2) | O1—C7—C6—C5 | -16.5 (2) |
| C8—C9—C10—C19 | 153.46 (14) | C10—C7—C6—C5 | 101.8 (2) |
| N1—C9—C10—C11 | 35.28 (16) | O1—C7—C6—C1 | 162.34 (14) |
| C13—C9—C10—C11 | 159.32 (14) | C10—C7—C6—C1 | -79.3 (2) |
| C8—C9—C10—C11 | -84.48 (15) | C5—C6—C1—C2 | -1.3 (3) |
| N1—C9—C10—C7 | 155.54 (13) | C7—C6—C1—C2 | 179.75 (16) |
| C13—C9—C10—C7 | -80.42 (16) | C7—O1—C8—O2 | 176.05 (16) |
| C8—C9—C10—C7 | 35.78 (15) | C7—O1—C8—C9 | -5.39 (18) |
| O1—C7—C10—C19 | -161.30 (12) | N1—C9—C8—O2 | 48.4 (2) |
| C6—C7—C10—C19 | 75.41 (18) | C13—C9—C8—O2 | -82.4 (2) |
| O1—C7—C10—C9 | -40.25 (15) | C10—C9—C8—O2 | 157.98 (18) |
| C6—C7—C10—C9 | -163.54 (14) | N1—C9—C8—O1 | -129.98 (15) |
| O1—C7—C10—C11 | 70.59 (16) | C13—C9—C8—O1 | 99.13 (16) |
| C6—C7—C10—C11 | -52.7 (2) | C10—C9—C8—O1 | -20.45 (17) |
| N1—C9—C13—C14 | -85.5 (2) | C21—N1—C12—C11 | 166.51 (16) |
| C10—C9—C13—C14 | 156.99 (17) | C9—N1—C12—C11 | 33.62 (19) |
| C8—C9—C13—C14 | 46.3 (2) | C10—C11—C12—N1 | -10.3 (2) |
| N1—C9—C13—C18 | 95.38 (19) | C6—C1—C2—C3 | 1.9 (3) |
| C10—C9—C13—C18 | -22.2 (2) | C6—C1—C2—C20 | -179.25 (18) |
| C8—C9—C13—C18 | -132.79 (17) | C13—C18—C17—C16 | 0.4 (3) |
| C18—N2—C19—O3 | -176.51 (18) | N2—C18—C17—C16 | -179.0 (2) |
| C18—N2—C19—C10 | 7.3 (3) | C1—C6—C5—C4 | -0.4 (3) |
| C9—C10—C19—O3 | 153.12 (16) | C7—C6—C5—C4 | 178.49 (19) |
| C11—C10—C19—O3 | 36.0 (2) | C1—C2—C3—C4 | -0.9 (3) |
| C7—C10—C19—O3 | -94.19 (19) | C20—C2—C3—C4 | -179.7 (2) |
| C9—C10—C19—N2 | -30.6 (2) | C18—C17—C16—C15 | -0.2 (3) |
| C11—C10—C19—N2 | -147.74 (16) | C2—C3—C4—C5 | -0.8 (3) |
| C7—C10—C19—N2 | 82.07 (18) | C6—C5—C4—C3 | 1.4 (3) |
| C14—C13—C18—C17 | 0.3 (3) | C17—C16—C15—C14 | -0.8 (4) |
| C9—C13—C18—C17 | 179.47 (17) | C13—C14—C15—C16 | 1.5 (4) |

Hydrogen-bond geometry (Å, °)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------------|----------|-------------|-------------|---------------|
| N2—H2A \cdots O3 ⁱ | 0.91 (2) | 1.93 (2) | 2.802 (2) | 159.6 (19) |
| C5—H5 \cdots O2 ⁱⁱ | 0.93 | 2.55 | 3.303 (3) | 138 |

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