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Ethyl *trans*-12-(pyridin-4-yl)-9,10-ethanoanthracene-11-carboxylateS. Chandrasekar,^a Prakash Sharma Om,^a
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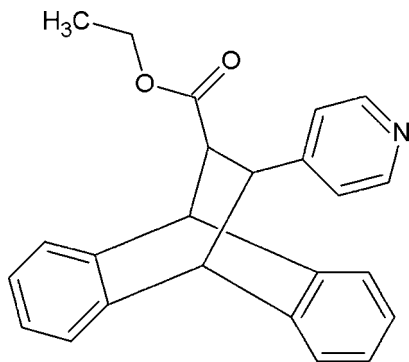
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.046; wR factor = 0.118; data-to-parameter ratio = 15.0.

In the title compound, $\text{C}_{24}\text{H}_{21}\text{NO}_2$, the residues at the central ethylene bridge are *trans* to each other. The dihedral angles between the pyridine and benzene rings are 67.09 (6) and 61.41 (5)°. In the crystal, centrosymmetrically related molecules are linked into dimers by pairs of $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For the biological activity of ester derivatives, see: Bi *et al.* (2012); Bartzatt *et al.* (2004); Anadu *et al.* (2006). For conformation studies, see: Nardelli (1983). For a related structure, see: Gnanamani & Ramanathan (2009).



Experimental

Crystal data

 $\text{C}_{24}\text{H}_{21}\text{NO}_2$ $M_r = 355.42$

Monoclinic, $P2_1/c$
 $a = 10.1733$ (19) Å
 $b = 11.156$ (2) Å
 $c = 16.361$ (3) Å
 $\beta = 90.877$ (3)°
 $V = 1856.6$ (6) Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 298$ K
 $0.40 \times 0.38 \times 0.20$ mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
 $T_{\min} = 0.969$, $T_{\max} = 0.984$

18677 measured reflections
3664 independent reflections
3105 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.118$
 $S = 1.05$
3664 reflections

245 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.17$ e Å⁻³
 $\Delta\rho_{\min} = -0.25$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{C18}-\text{H18}\cdots\text{O1}^i$ | 0.93 | 2.55 | 3.2612 (18) | 134 |

Symmetry code: (i) $-x + 1, -y + 2, -z + 2$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2010); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2010); data reduction: *CrysAlis RED*; 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: *PLATON* (Spek, 2009).

CRR thanks DST-FIST for the single-crystal X-ray facility at the Department of Chemistry, Pondicherry University, Pondicherry.

Supporting information for this paper is available from the IUCr electronic archives (Reference: BT6931).

References

- Anadu, N. O., Davisson, V. J. & Cushman, M. (2006). *J. Med. Chem.* **49**, 3897–3905.
Bartzatt, R., Cirillo, S. L. & Cirillo, J. D. (2004). *Physiol. Chem. Phys. Med. NMR*, **36**, 85–94.
Bi, Y., Xu, J., Sun, F., Wu, X., Ye, W., Sun, Y. & Huang, W. (2012). *Molecules*, **17**, 8832–8841.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Gnanamani, E. & Ramanathan, C. R. (2009). *Tetrahedron Asymmetry*, **20**, 2211–2215.
Nardelli, M. (1983). *Acta Cryst.* **C39**, 1141–1142.
Oxford Diffraction (2010). *CrysAlis PRO*, *CrysAlis RED* and *CrysAlis CCD*. Oxford Diffraction Ltd, Yarnton, England.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supporting information

Acta Cryst. (2014). E70, o512 [doi:10.1107/S1600536814006588]

Ethyl *trans*-12-(pyridin-4-yl)-9,10-ethanoanthracene-11-carboxylate

S. Chandrasekar, Prakash Sharma Om, V. Srinivasapriyan, M. SureshKumar and C. R. Ramanathan

S1. Comment

Ester derivatives of many compounds exhibit a variety of pharmacological properties, for example anticancer, antitumor and antimicrobial activities (Anadu *et al.*, 2006; Bi *et al.*, 2012; Bartzatt *et al.*, 2004). In view of their importance, the title compound was synthesized and we report herein on its crystal structure. In the title molecule (Fig. 1) the fused tricyclic rings [DS (C7) = 0.0051 (1) Å and D2 (C7—C6) = 0.2248 (1) Å], [DS (C7) = 0.0135 (8) Å and D2 (C7—C6) = 0.2358 (6) Å] and [DS (C7) = 0.0126 (9) Å and D2 (C7—C6) = 0.2543 (7) Å] adopt a boat conformation which can be defined by the above asymmetry parameters (Nardelli, 1983). The torsion angles H7—C7—C8—H8 = -65.81 (15)° and H8—C8—C9—H9 = 129.38 (12)°, define the ring fusions involving the fused tricyclic ring system of the ethanoanthracene moiety. The C22—O1 distance [1.326 (2) Å] shows a partial double-bond character and so the C23 maintains planarity with C22, O2 and C9. In the crystal, pairs of centrosymmetrically related molecules are linked into dimers by C18—H18···O1 hydrogen bonds (Fig. 2).

S2. Experimental

Anthracene (5.34 g, 30 mmol) and 3-(pyridine-4-yl)-acrylic acid ethyl ester (4.4g, 25 mmol) were taken in round bottom flask containing distilled dichloromethane (100 ml). To this mixture anhydrous AlCl₃ (6.6 g, 50 mmol) was added and stirred at 0 °C for 48 h followed by stirring the reaction mixture at room temperature for 10 h. The obtained dark black solution was poured into water, the organic layer was separated and the aqueous layer was extracted with ether. The crude material was purified through column chromatography using hexane and ethyl acetate in the ratio of 9:1 as eluent. Yield: 5.7 g, (65%).

S3. Refinement

All H atoms were positioned geometrically, with C—H = 0.93–0.97 Å and constrained to ride on their parent atom, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C})$ for other H atoms.

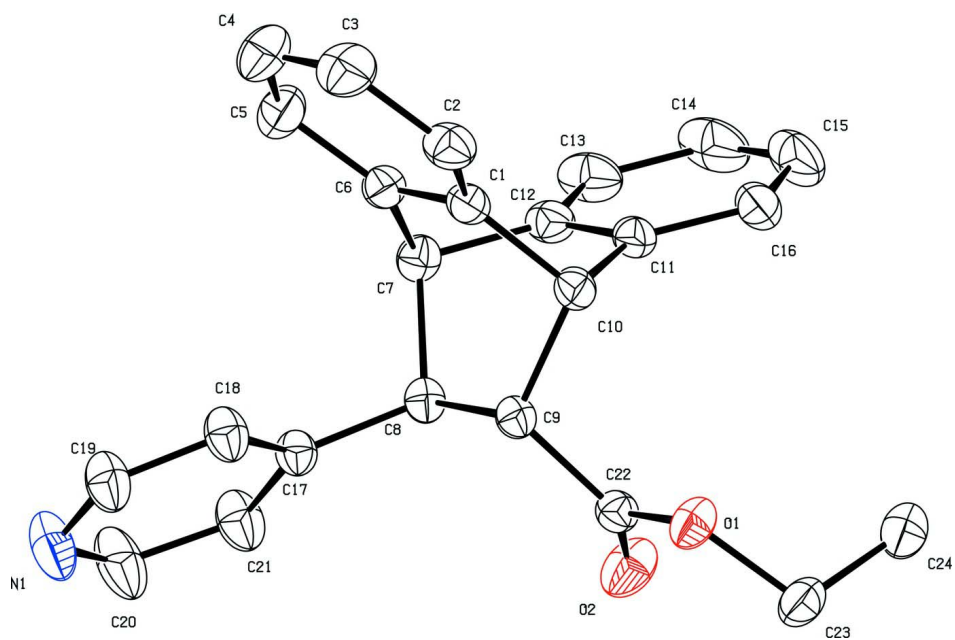


Figure 1

The molecular structure of the title compound, Displacement ellipsoids are drawn at the 30% probability level, H atoms have been omitted for clarity.

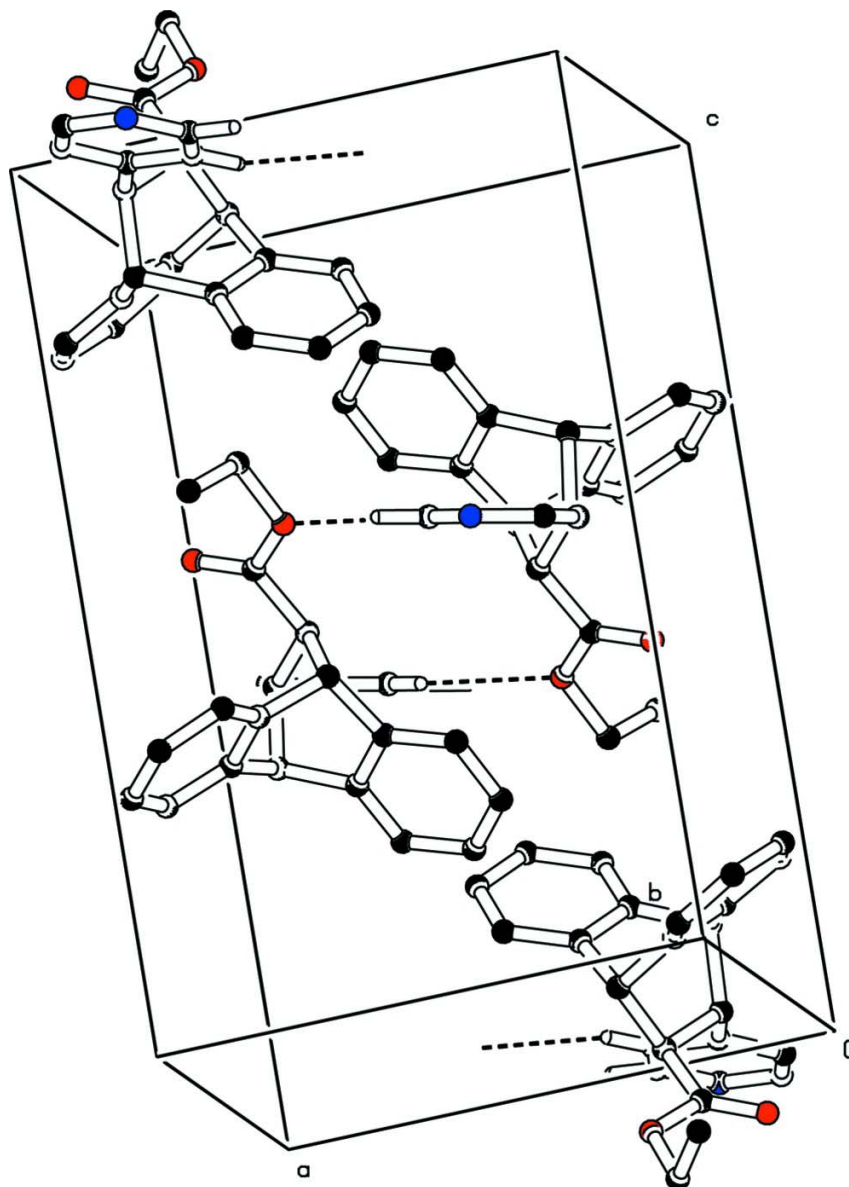


Figure 2

Crystal packing of the title compound, Hydrogen bonds are shown as dashed lines. For the sake of clarity, H atoms not involved in the interactions have been omitted.

(I)

Crystal data

$C_{24}H_{21}NO_2$

$M_r = 355.42$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 10.1733\ (19)\ \text{\AA}$

$b = 11.156\ (2)\ \text{\AA}$

$c = 16.361\ (3)\ \text{\AA}$

$\beta = 90.877\ (3)^\circ$

$V = 1856.6\ (6)\ \text{\AA}^3$

$Z = 4$

$F(000) = 752$

$D_x = 1.272\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 9754 reflections

$\theta = 2.2\text{--}26.0^\circ$

$\mu = 0.08\ \text{mm}^{-1}$

$T = 298$ K $0.40 \times 0.38 \times 0.20$ mm
 Block, colourless

Data collection

| | |
|--|--|
| Oxford Diffraction Xcalibur Eos diffractometer | 18677 measured reflections |
| Radiation source: fine-focus sealed tube | 3664 independent reflections |
| Graphite monochromator | 3105 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 15.9821 pixels mm ⁻¹ | $R_{\text{int}} = 0.027$ |
| ω scans | $\theta_{\text{max}} = 26.1^\circ$, $\theta_{\text{min}} = 2.0^\circ$ |
| Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Oxford Diffraction, 2010) | $h = -12 \rightarrow 12$ |
| $T_{\text{min}} = 0.969$, $T_{\text{max}} = 0.984$ | $k = -13 \rightarrow 13$ |
| | $l = -20 \rightarrow 20$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.046$ | H-atom parameters constrained |
| $wR(F^2) = 0.118$ | $w = 1/[\sigma^2(F_o^2) + (0.0561P)^2 + 0.4341P]$ |
| $S = 1.05$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 3664 reflections | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 245 parameters | $\Delta\rho_{\text{max}} = 0.17 \text{ e } \text{\AA}^{-3}$ |
| 0 restraints | $\Delta\rho_{\text{min}} = -0.25 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | |

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|--------------|--------------|--------------|----------------------------------|
| C1 | 0.59145 (13) | 0.92171 (12) | 0.85231 (8) | 0.0392 (3) |
| C2 | 0.46282 (15) | 0.90612 (15) | 0.82600 (10) | 0.0502 (4) |
| H2 | 0.4091 | 0.8500 | 0.8510 | 0.060* |
| C3 | 0.41498 (17) | 0.97553 (18) | 0.76167 (12) | 0.0649 (5) |
| H3 | 0.3289 | 0.9652 | 0.7430 | 0.078* |
| C4 | 0.49392 (19) | 1.05918 (18) | 0.72543 (11) | 0.0685 (5) |
| H4 | 0.4610 | 1.1050 | 0.6823 | 0.082* |
| C5 | 0.62142 (17) | 1.07578 (16) | 0.75239 (10) | 0.0565 (4) |
| H5 | 0.6739 | 1.1334 | 0.7280 | 0.068* |
| C6 | 0.67128 (14) | 1.00685 (13) | 0.81564 (8) | 0.0407 (3) |
| C7 | 0.80801 (13) | 1.01204 (13) | 0.85311 (9) | 0.0406 (3) |
| H7 | 0.8639 | 1.0697 | 0.8248 | 0.049* |
| C8 | 0.79534 (12) | 1.04310 (11) | 0.94622 (8) | 0.0354 (3) |
| H8 | 0.8826 | 1.0330 | 0.9715 | 0.042* |

| | | | | |
|------|--------------|--------------|--------------|------------|
| C9 | 0.70331 (12) | 0.95000 (12) | 0.98565 (8) | 0.0341 (3) |
| H9 | 0.6244 | 0.9919 | 1.0039 | 0.041* |
| C10 | 0.66015 (13) | 0.85398 (12) | 0.92048 (8) | 0.0381 (3) |
| H10 | 0.6035 | 0.7923 | 0.9440 | 0.046* |
| C11 | 0.78412 (14) | 0.80130 (13) | 0.88616 (9) | 0.0425 (3) |
| C12 | 0.86419 (14) | 0.88680 (14) | 0.85040 (9) | 0.0442 (3) |
| C13 | 0.98283 (16) | 0.85354 (18) | 0.81716 (11) | 0.0623 (5) |
| H13 | 1.0384 | 0.9106 | 0.7947 | 0.075* |
| C14 | 1.0172 (2) | 0.7333 (2) | 0.81801 (14) | 0.0812 (7) |
| H14 | 1.0962 | 0.7096 | 0.7951 | 0.097* |
| C15 | 0.9370 (2) | 0.6489 (2) | 0.85202 (14) | 0.0788 (7) |
| H15 | 0.9615 | 0.5686 | 0.8511 | 0.095* |
| C16 | 0.82018 (18) | 0.68175 (15) | 0.88763 (11) | 0.0582 (5) |
| H16 | 0.7669 | 0.6247 | 0.9121 | 0.070* |
| C17 | 0.75608 (13) | 1.17233 (12) | 0.95790 (8) | 0.0381 (3) |
| C18 | 0.62967 (14) | 1.21560 (13) | 0.94575 (10) | 0.0475 (4) |
| H18 | 0.5619 | 1.1633 | 0.9316 | 0.057* |
| C19 | 0.60451 (16) | 1.33606 (14) | 0.95456 (11) | 0.0568 (4) |
| H19 | 0.5186 | 1.3623 | 0.9461 | 0.068* |
| C20 | 0.81530 (19) | 1.37470 (16) | 0.98575 (15) | 0.0766 (6) |
| H20 | 0.8812 | 1.4293 | 0.9993 | 0.092* |
| C21 | 0.85033 (16) | 1.25592 (14) | 0.97912 (12) | 0.0578 (4) |
| H21 | 0.9368 | 1.2323 | 0.9889 | 0.069* |
| C22 | 0.76667 (13) | 0.88949 (12) | 1.05943 (8) | 0.0371 (3) |
| C23 | 0.73365 (16) | 0.73634 (15) | 1.15837 (9) | 0.0513 (4) |
| H23A | 0.6605 | 0.7091 | 1.1909 | 0.062* |
| H23B | 0.7918 | 0.7833 | 1.1933 | 0.062* |
| C24 | 0.8059 (2) | 0.63115 (16) | 1.12588 (11) | 0.0657 (5) |
| H24A | 0.7502 | 0.5882 | 1.0881 | 0.099* |
| H24B | 0.8310 | 0.5792 | 1.1702 | 0.099* |
| H24C | 0.8831 | 0.6581 | 1.0983 | 0.099* |
| N1 | 0.69472 (15) | 1.41714 (12) | 0.97428 (11) | 0.0713 (5) |
| O1 | 0.68494 (10) | 0.81027 (9) | 1.09130 (6) | 0.0474 (3) |
| O2 | 0.87508 (11) | 0.90811 (11) | 1.08561 (7) | 0.0628 (3) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|-------------|--------------|
| C1 | 0.0418 (7) | 0.0369 (7) | 0.0388 (7) | 0.0032 (6) | -0.0034 (6) | -0.0068 (6) |
| C2 | 0.0442 (8) | 0.0539 (9) | 0.0522 (9) | 0.0000 (7) | -0.0074 (7) | -0.0095 (7) |
| C3 | 0.0498 (9) | 0.0783 (13) | 0.0659 (11) | 0.0112 (9) | -0.0219 (8) | -0.0064 (10) |
| C4 | 0.0721 (12) | 0.0729 (12) | 0.0598 (11) | 0.0150 (10) | -0.0192 (9) | 0.0128 (9) |
| C5 | 0.0622 (10) | 0.0562 (10) | 0.0511 (9) | 0.0068 (8) | -0.0028 (8) | 0.0117 (8) |
| C6 | 0.0442 (8) | 0.0404 (7) | 0.0374 (7) | 0.0065 (6) | -0.0001 (6) | -0.0016 (6) |
| C7 | 0.0388 (7) | 0.0416 (8) | 0.0416 (7) | 0.0001 (6) | 0.0052 (6) | 0.0039 (6) |
| C8 | 0.0302 (6) | 0.0331 (7) | 0.0428 (7) | -0.0015 (5) | -0.0013 (5) | 0.0013 (6) |
| C9 | 0.0318 (6) | 0.0324 (7) | 0.0381 (7) | -0.0005 (5) | -0.0001 (5) | -0.0011 (5) |
| C10 | 0.0406 (7) | 0.0328 (7) | 0.0408 (7) | -0.0045 (5) | -0.0042 (6) | -0.0010 (6) |

| | | | | | | |
|-----|-------------|-------------|-------------|-------------|--------------|--------------|
| C11 | 0.0484 (8) | 0.0386 (8) | 0.0403 (7) | 0.0069 (6) | -0.0105 (6) | -0.0065 (6) |
| C12 | 0.0421 (8) | 0.0510 (9) | 0.0393 (7) | 0.0092 (6) | -0.0030 (6) | -0.0072 (6) |
| C13 | 0.0464 (9) | 0.0837 (13) | 0.0567 (10) | 0.0132 (9) | 0.0010 (7) | -0.0188 (9) |
| C14 | 0.0606 (11) | 0.1010 (17) | 0.0817 (14) | 0.0389 (12) | -0.0100 (10) | -0.0405 (13) |
| C15 | 0.0844 (14) | 0.0631 (12) | 0.0880 (14) | 0.0378 (11) | -0.0288 (12) | -0.0299 (11) |
| C16 | 0.0730 (11) | 0.0420 (9) | 0.0589 (10) | 0.0140 (8) | -0.0235 (8) | -0.0121 (7) |
| C17 | 0.0380 (7) | 0.0338 (7) | 0.0426 (7) | -0.0026 (6) | 0.0003 (6) | 0.0013 (6) |
| C18 | 0.0387 (7) | 0.0370 (8) | 0.0668 (10) | -0.0028 (6) | -0.0044 (7) | -0.0008 (7) |
| C19 | 0.0484 (9) | 0.0404 (8) | 0.0813 (12) | 0.0056 (7) | -0.0079 (8) | -0.0006 (8) |
| C20 | 0.0603 (11) | 0.0398 (9) | 0.1291 (19) | -0.0094 (8) | -0.0204 (11) | -0.0138 (10) |
| C21 | 0.0433 (8) | 0.0423 (9) | 0.0873 (13) | -0.0028 (7) | -0.0129 (8) | -0.0065 (8) |
| C22 | 0.0372 (7) | 0.0355 (7) | 0.0385 (7) | -0.0018 (5) | -0.0013 (5) | -0.0025 (6) |
| C23 | 0.0600 (9) | 0.0524 (9) | 0.0414 (8) | -0.0006 (7) | -0.0028 (7) | 0.0126 (7) |
| C24 | 0.0885 (13) | 0.0532 (10) | 0.0555 (10) | 0.0116 (9) | 0.0022 (9) | 0.0108 (8) |
| N1 | 0.0656 (10) | 0.0358 (7) | 0.1119 (14) | 0.0022 (7) | -0.0146 (9) | -0.0070 (8) |
| O1 | 0.0444 (6) | 0.0500 (6) | 0.0476 (6) | -0.0064 (5) | -0.0044 (4) | 0.0145 (5) |
| O2 | 0.0502 (7) | 0.0725 (8) | 0.0651 (7) | -0.0186 (6) | -0.0210 (5) | 0.0209 (6) |

Geometric parameters (Å, °)

| | | | |
|----------|-------------|------------|-------------|
| C1—C2 | 1.382 (2) | C13—C14 | 1.386 (3) |
| C1—C6 | 1.392 (2) | C13—H13 | 0.9300 |
| C1—C10 | 1.5097 (19) | C14—C15 | 1.370 (3) |
| C2—C3 | 1.389 (2) | C14—H14 | 0.9300 |
| C2—H2 | 0.9300 | C15—C16 | 1.381 (3) |
| C3—C4 | 1.372 (3) | C15—H15 | 0.9300 |
| C3—H3 | 0.9300 | C16—H16 | 0.9300 |
| C4—C5 | 1.376 (3) | C17—C21 | 1.378 (2) |
| C4—H4 | 0.9300 | C17—C18 | 1.385 (2) |
| C5—C6 | 1.380 (2) | C18—C19 | 1.376 (2) |
| C5—H5 | 0.9300 | C18—H18 | 0.9300 |
| C6—C7 | 1.513 (2) | C19—N1 | 1.325 (2) |
| C7—C12 | 1.510 (2) | C19—H19 | 0.9300 |
| C7—C8 | 1.5695 (19) | C20—N1 | 1.326 (2) |
| C7—H7 | 0.9800 | C20—C21 | 1.377 (2) |
| C8—C17 | 1.5089 (19) | C20—H20 | 0.9300 |
| C8—C9 | 1.5460 (17) | C21—H21 | 0.9300 |
| C8—H8 | 0.9800 | C22—O2 | 1.1952 (17) |
| C9—C22 | 1.5180 (18) | C22—O1 | 1.3258 (16) |
| C9—C10 | 1.5693 (18) | C23—O1 | 1.4538 (17) |
| C9—H9 | 0.9800 | C23—C24 | 1.487 (2) |
| C10—C11 | 1.508 (2) | C23—H23A | 0.9700 |
| C10—H10 | 0.9800 | C23—H23B | 0.9700 |
| C11—C16 | 1.383 (2) | C24—H24A | 0.9600 |
| C11—C12 | 1.389 (2) | C24—H24B | 0.9600 |
| C12—C13 | 1.382 (2) | C24—H24C | 0.9600 |
| C2—C1—C6 | 120.50 (14) | C13—C12—C7 | 126.37 (16) |

| | | | |
|--------------|--------------|-----------------|-------------|
| C2—C1—C10 | 126.33 (13) | C11—C12—C7 | 113.46 (12) |
| C6—C1—C10 | 113.17 (12) | C12—C13—C14 | 118.5 (2) |
| C1—C2—C3 | 119.01 (16) | C12—C13—H13 | 120.7 |
| C1—C2—H2 | 120.5 | C14—C13—H13 | 120.7 |
| C3—C2—H2 | 120.5 | C15—C14—C13 | 121.14 (18) |
| C4—C3—C2 | 120.41 (16) | C15—C14—H14 | 119.4 |
| C4—C3—H3 | 119.8 | C13—C14—H14 | 119.4 |
| C2—C3—H3 | 119.8 | C14—C15—C16 | 120.74 (18) |
| C3—C4—C5 | 120.54 (16) | C14—C15—H15 | 119.6 |
| C3—C4—H4 | 119.7 | C16—C15—H15 | 119.6 |
| C5—C4—H4 | 119.7 | C15—C16—C11 | 118.55 (19) |
| C4—C5—C6 | 119.96 (17) | C15—C16—H16 | 120.7 |
| C4—C5—H5 | 120.0 | C11—C16—H16 | 120.7 |
| C6—C5—H5 | 120.0 | C21—C17—C18 | 116.18 (13) |
| C5—C6—C1 | 119.57 (14) | C21—C17—C8 | 119.60 (13) |
| C5—C6—C7 | 127.44 (14) | C18—C17—C8 | 124.18 (12) |
| C1—C6—C7 | 112.98 (12) | C19—C18—C17 | 119.94 (14) |
| C12—C7—C6 | 107.38 (12) | C19—C18—H18 | 120.0 |
| C12—C7—C8 | 105.63 (11) | C17—C18—H18 | 120.0 |
| C6—C7—C8 | 108.25 (11) | N1—C19—C18 | 124.26 (15) |
| C12—C7—H7 | 111.8 | N1—C19—H19 | 117.9 |
| C6—C7—H7 | 111.8 | C18—C19—H19 | 117.9 |
| C8—C7—H7 | 111.8 | N1—C20—C21 | 124.93 (16) |
| C17—C8—C9 | 115.20 (11) | N1—C20—H20 | 117.5 |
| C17—C8—C7 | 111.08 (11) | C21—C20—H20 | 117.5 |
| C9—C8—C7 | 108.42 (10) | C20—C21—C17 | 119.42 (15) |
| C17—C8—H8 | 107.3 | C20—C21—H21 | 120.3 |
| C9—C8—H8 | 107.3 | C17—C21—H21 | 120.3 |
| C7—C8—H8 | 107.3 | O2—C22—O1 | 123.76 (13) |
| C22—C9—C8 | 112.21 (10) | O2—C22—C9 | 125.88 (13) |
| C22—C9—C10 | 110.35 (11) | O1—C22—C9 | 110.36 (11) |
| C8—C9—C10 | 109.87 (11) | O1—C23—C24 | 110.02 (13) |
| C22—C9—H9 | 108.1 | O1—C23—H23A | 109.7 |
| C8—C9—H9 | 108.1 | C24—C23—H23A | 109.7 |
| C10—C9—H9 | 108.1 | O1—C23—H23B | 109.7 |
| C11—C10—C1 | 107.48 (11) | C24—C23—H23B | 109.7 |
| C11—C10—C9 | 106.99 (11) | H23A—C23—H23B | 108.2 |
| C1—C10—C9 | 106.37 (11) | C23—C24—H24A | 109.5 |
| C11—C10—H10 | 111.9 | C23—C24—H24B | 109.5 |
| C1—C10—H10 | 111.9 | H24A—C24—H24B | 109.5 |
| C9—C10—H10 | 111.9 | C23—C24—H24C | 109.5 |
| C16—C11—C12 | 120.81 (15) | H24A—C24—H24C | 109.5 |
| C16—C11—C10 | 126.33 (15) | H24B—C24—H24C | 109.5 |
| C12—C11—C10 | 112.86 (12) | C19—N1—C20 | 115.26 (14) |
| C13—C12—C11 | 120.17 (15) | C22—O1—C23 | 117.80 (11) |
| C6—C1—C2—C3 | 0.9 (2) | C16—C11—C12—C13 | -1.3 (2) |
| C10—C1—C2—C3 | -179.47 (14) | C10—C11—C12—C13 | 178.93 (13) |

| | | | |
|----------------|--------------|-----------------|--------------|
| C1—C2—C3—C4 | -0.7 (3) | C16—C11—C12—C7 | 178.95 (13) |
| C2—C3—C4—C5 | -0.2 (3) | C10—C11—C12—C7 | -0.77 (17) |
| C3—C4—C5—C6 | 0.9 (3) | C6—C7—C12—C13 | 126.43 (16) |
| C4—C5—C6—C1 | -0.7 (2) | C8—C7—C12—C13 | -118.21 (16) |
| C4—C5—C6—C7 | 179.87 (16) | C6—C7—C12—C11 | -53.89 (15) |
| C2—C1—C6—C5 | -0.2 (2) | C8—C7—C12—C11 | 61.47 (14) |
| C10—C1—C6—C5 | -179.89 (13) | C11—C12—C13—C14 | 2.1 (2) |
| C2—C1—C6—C7 | 179.33 (13) | C7—C12—C13—C14 | -178.20 (15) |
| C10—C1—C6—C7 | -0.36 (17) | C12—C13—C14—C15 | -1.0 (3) |
| C5—C6—C7—C12 | -126.13 (16) | C13—C14—C15—C16 | -1.0 (3) |
| C1—C6—C7—C12 | 54.38 (15) | C14—C15—C16—C11 | 1.8 (3) |
| C5—C6—C7—C8 | 120.26 (16) | C12—C11—C16—C15 | -0.6 (2) |
| C1—C6—C7—C8 | -59.23 (15) | C10—C11—C16—C15 | 179.04 (15) |
| C12—C7—C8—C17 | 172.86 (11) | C9—C8—C17—C21 | 135.65 (15) |
| C6—C7—C8—C17 | -72.38 (14) | C7—C8—C17—C21 | -100.59 (16) |
| C12—C7—C8—C9 | -59.59 (13) | C9—C8—C17—C18 | -46.84 (19) |
| C6—C7—C8—C9 | 55.17 (14) | C7—C8—C17—C18 | 76.93 (17) |
| C17—C8—C9—C22 | -109.03 (13) | C21—C17—C18—C19 | 0.4 (2) |
| C7—C8—C9—C22 | 125.81 (12) | C8—C17—C18—C19 | -177.20 (15) |
| C17—C8—C9—C10 | 127.81 (12) | C17—C18—C19—N1 | 0.2 (3) |
| C7—C8—C9—C10 | 2.65 (14) | N1—C20—C21—C17 | 1.0 (4) |
| C2—C1—C10—C11 | 125.88 (15) | C18—C17—C21—C20 | -0.9 (3) |
| C6—C1—C10—C11 | -54.46 (15) | C8—C17—C21—C20 | 176.79 (17) |
| C2—C1—C10—C9 | -119.80 (15) | C8—C9—C22—O2 | -0.6 (2) |
| C6—C1—C10—C9 | 59.86 (14) | C10—C9—C22—O2 | 122.24 (16) |
| C22—C9—C10—C11 | -68.66 (14) | C8—C9—C22—O1 | -179.85 (11) |
| C8—C9—C10—C11 | 55.59 (14) | C10—C9—C22—O1 | -56.96 (14) |
| C22—C9—C10—C1 | 176.69 (11) | C18—C19—N1—C20 | -0.1 (3) |
| C8—C9—C10—C1 | -59.07 (13) | C21—C20—N1—C19 | -0.4 (3) |
| C1—C10—C11—C16 | -124.66 (15) | O2—C22—O1—C23 | -4.4 (2) |
| C9—C10—C11—C16 | 121.43 (15) | C9—C22—O1—C23 | 174.85 (12) |
| C1—C10—C11—C12 | 55.04 (15) | C24—C23—O1—C22 | -83.74 (17) |
| C9—C10—C11—C12 | -58.87 (15) | | |

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------|-------|-------------|-------------|---------------|
| C18—H18 \cdots O1 ⁱ | 0.93 | 2.55 | 3.2612 (18) | 134 |

Symmetry code: (i) $-x+1, -y+2, -z+2$.