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5-Methyl-3-phenylisoxazole-4-carboxylic acid

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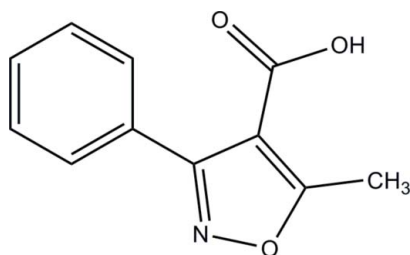
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.039; wR factor = 0.111; data-to-parameter ratio = 12.4.

In the title compound, $\text{C}_{11}\text{H}_9\text{NO}_3$, the phenyl and isoxazole rings form a dihedral angle of 56.64 (8°). The carboxy group is almost in the same plane as the isoxazole ring with a $\text{C}-\text{C}-\text{C}-\text{O}$ torsion angle of -3.3 (2°). In the crystal, pairs of $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into head-to-head dimers. $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds and $\pi-\pi$ stacking interactions between phenyl rings [centroid-centroid distance = 3.9614 (17)Å] link the dimers into a three-dimensional network.

Related literature

For the biological and pharmaceutical importance of isoxazoles, see: Basappa *et al.*, (2003); Conti *et al.* (1998); Kang *et al.* (2000); Lee *et al.* (2009); Shin *et al.* (2005); Stevens & Albizati (1984). For bond-length and angle data in related structures, see: Wolf *et al.* (1995); Chandra *et al.*, (2013).



Experimental

Crystal data

 $\text{C}_{11}\text{H}_9\text{NO}_3$ $M_r = 203.19$

Monoclinic, $P2_1/n$
 $a = 11.953$ (4) Å
 $b = 5.981$ (2) Å
 $c = 14.142$ (5) Å
 $\beta = 105.548$ (6°)
 $V = 974.0$ (6) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 273$ K
 $0.30 \times 0.25 \times 0.20$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 8619 measured reflections

1712 independent reflections
 1558 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.111$
 $S = 1.05$
 1712 reflections

138 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.19$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.14$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|-------|-------------|-------------|---------------|
| $\text{O14}-\text{H14}\cdots\text{O15}^{\text{i}}$ | 0.82 | 1.81 | 2.6252 (18) | 172 |
| $\text{C11}-\text{H11A}\cdots\text{N8}^{\text{ii}}$ | 0.96 | 2.51 | 3.427 (2) | 159 |

Symmetry codes: (i) $-x + 2, -y, -z$; (ii) $-x + \frac{3}{2}, y - \frac{1}{2}, -z - \frac{1}{2}$.

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); 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.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2504).

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supporting information

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5-Methyl-3-phenylisoxazole-4-carboxylic acid

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S1. Comment

Isoxazole derivatives bearing various substituents are known to have diverse biological and pharmaceutical activities; such as anti-tumor (Kang *et al.*, 2000), antiviral (Lee *et al.*, 2009), hypoglycemic (Conti *et al.*, 1998), antifungal (Basappa *et al.*, 2003) and anti-HIV activities (Shin *et al.*, 2005). In addition, isoxazoles and related compounds have attracted much interest because of their fungicidal, plant-growth regulating and antibacterial activities (Stevens & Albizati, 1984). As part of our interest in these compounds and our extensive background on isoxazole derivatives, we have synthesized the title compound to study its crystal structure.

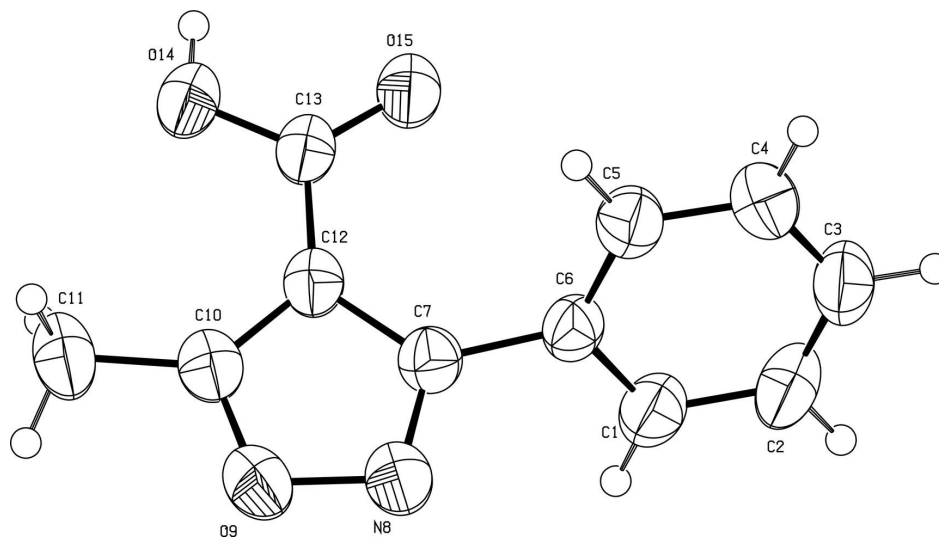
Fig. 1 presents an ellipsoid plot of the title compound (I). The (C7/N8/O9/C10/C12) isoxazole ring is in Syn-Clinal conformation with respect to the (C1-C2-C3-C4-C5-C6) phenyl ring, as indicated by the (C1-C6-C7-N8) torsion angle of $-54.40(19)^\circ$. The carboxylic acid group at C12 is almost in the same plane as the isoxazole ring (C7-C12-C13-O15 torsion angle = $-3.3(2)^\circ$). The bond lengths and angles are within normal ranges and are comparable to related structure (Wolf *et al.*, 1995 & Chandra *et al.*, 2013). The crystal structure is stabilized by O—H \cdots O bonds (Table 1), which define head to head dimers, and weaker C—H \cdots N bonds (Table 1), thus defining planes parallel to $(\bar{1}01)$ (Fig 2). Finally, there are $\pi\cdots\pi$ stacking interactions between phenyl rings with Cg \cdots Cg[1-x,1-y,-z] and slippage displacement distances of 3.9614 (17)Å and 1.284Å respectively (Fig 3) which link planes into a 3D structure.

S2. Experimental

A mixture of benzaldehyde oxime (1 mmol), ethyl acetoacetate (2 mmol) and anhydrous zinc chloride (0.1 mmol) were taken in a 10 ml round bottomed flask and the contents were gradually heated to 60°C without any solvent for about one hour. After completion of the reaction (as indicated by TLC), the mixture was cooled to room temperature and ethanol was added with stirring for about 30 min. The solid ethyl 5-methyl-3-phenylisoxazole-4-carboxylate thus obtained was treated with 5% NaOH (10 ml) at room temperature for about 4hr. After completion of the reaction (as indicated by TLC), the reaction mixture was acidified with 2 N HCl. The solids thus obtained were filtered and recrystallized from hot ethanol to get crystals of the title compound.

S3. Refinement

H atoms were placed at idealized positions and allowed to ride on their parent atoms with C—H distances in the range of 0.93 to 0.96 Å; $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier atom})$ for all H atoms.

**Figure 1**

Perspective diagram of the molecule with 50% probability displacement ellipsoids.

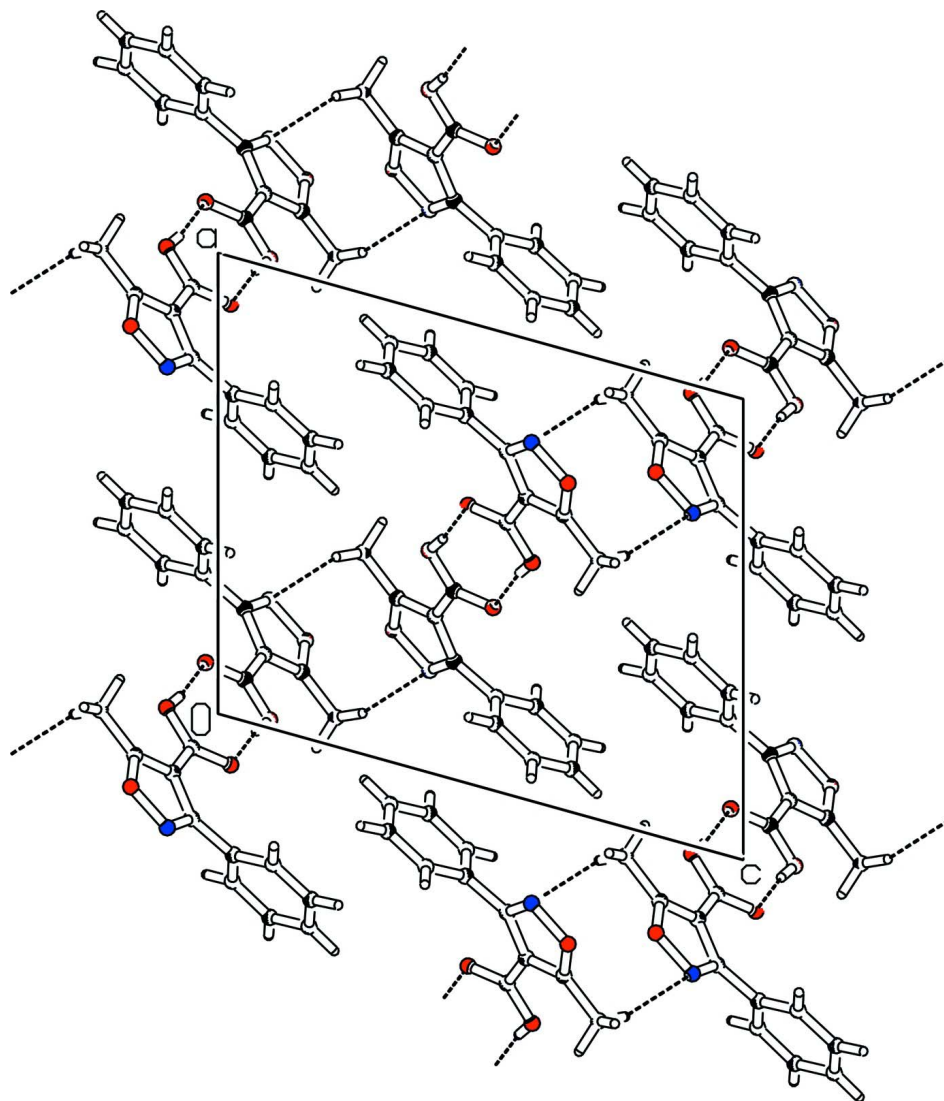
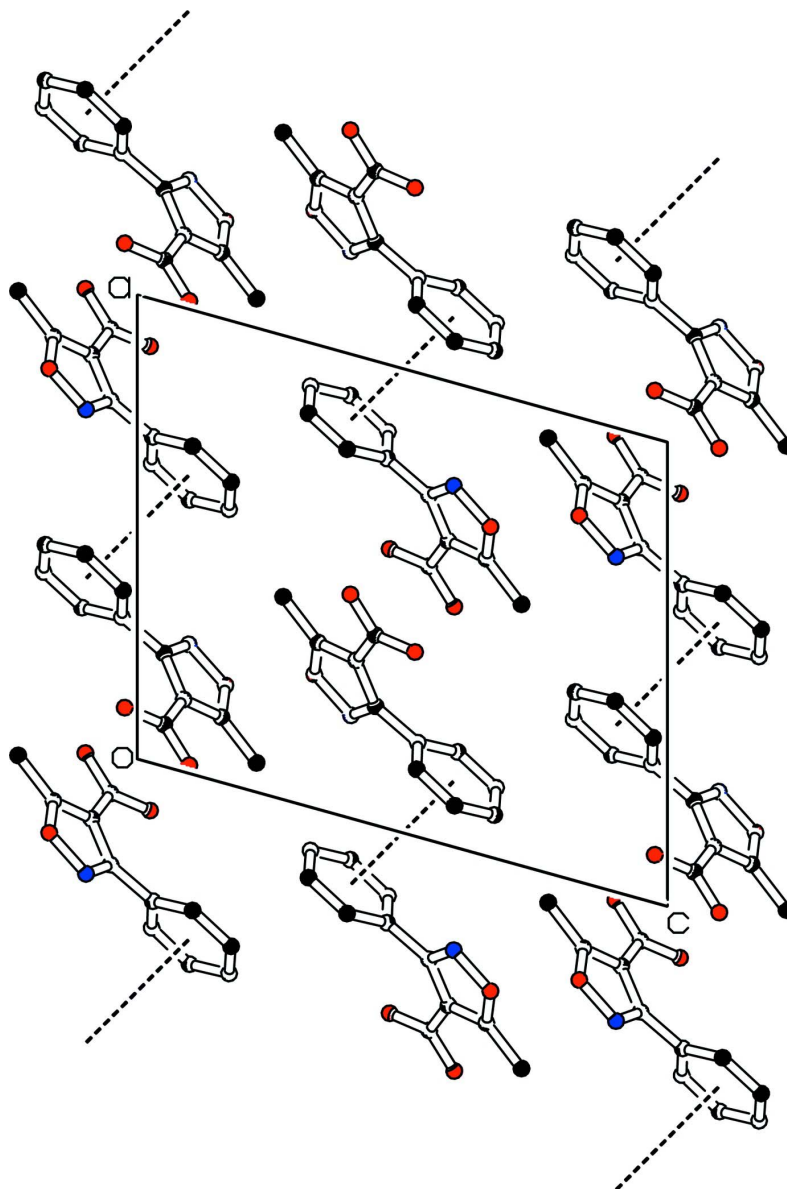


Figure 2

Packing diagram of the molecule viewed down the 'b' axis, showing the H-bonded dimers.

**Figure 3**

Packing diagram of the molecule viewed down the 'b' axis, showing the π - π interactions.

5-Methyl-3-phenylisoxazole-4-carboxylic acid

Crystal data

$C_{11}H_9NO_3$

$M_r = 203.19$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 11.953\ (4)\ \text{\AA}$

$b = 5.981\ (2)\ \text{\AA}$

$c = 14.142\ (5)\ \text{\AA}$

$\beta = 105.548\ (6)^\circ$

$V = 974.0\ (6)\ \text{\AA}^3$

$Z = 4$

$F(000) = 424$

$D_x = 1.386\ \text{Mg m}^{-3}$

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

Cell parameters from 1712 reflections

$\theta = 2.0\text{--}25.0^\circ$

$\mu = 0.10\ \text{mm}^{-1}$

$T = 273\ \text{K}$

Block, yellow

$0.30 \times 0.25 \times 0.20\ \text{mm}$

Data collection

Bruker APEXII CCD area-detector
diffractometer
 ω and φ scans
8619 measured reflections
1712 independent reflections
1558 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$
 $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.0^\circ$
 $h = -14 \rightarrow 14$
 $k = -7 \rightarrow 7$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.111$
 $S = 1.05$
1712 reflections
138 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
 $w = 1/[\sigma^2(F_o^2) + (0.0647P)^2 + 0.1799P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.19 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.14 \text{ e } \text{\AA}^{-3}$
Extinction correction: *SHELXL97* (Sheldrick,
2008), $\text{FC}^* = \text{KFC}[1 + 0.001\text{XFC}^2\Lambda^3/\text{SIN}(2\Theta)]^{-1/4}$
Extinction coefficient: 0.078 (6)

Special details

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

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|---------------|----------------------------------|
| O9 | 0.78858 (10) | 0.77608 (19) | -0.16618 (8) | 0.0644 (4) |
| O14 | 0.98209 (9) | 0.19333 (19) | -0.09796 (8) | 0.0626 (4) |
| O15 | 0.89662 (9) | 0.16156 (18) | 0.02382 (7) | 0.0583 (4) |
| N8 | 0.72219 (12) | 0.7544 (2) | -0.09692 (10) | 0.0627 (5) |
| C1 | 0.70696 (13) | 0.6540 (3) | 0.10434 (12) | 0.0577 (5) |
| C2 | 0.65298 (14) | 0.6027 (3) | 0.17680 (13) | 0.0667 (6) |
| C3 | 0.59319 (14) | 0.4050 (3) | 0.17315 (12) | 0.0646 (6) |
| C4 | 0.58949 (14) | 0.2546 (3) | 0.09855 (13) | 0.0634 (5) |
| C5 | 0.64525 (13) | 0.3017 (3) | 0.02718 (11) | 0.0556 (5) |
| C6 | 0.70323 (11) | 0.5035 (2) | 0.02904 (9) | 0.0458 (4) |
| C7 | 0.75633 (11) | 0.5675 (2) | -0.05041 (10) | 0.0465 (4) |
| C10 | 0.85935 (12) | 0.6006 (2) | -0.15866 (10) | 0.0503 (4) |
| C11 | 0.93670 (14) | 0.6030 (3) | -0.22477 (11) | 0.0643 (6) |
| C12 | 0.84386 (10) | 0.4605 (2) | -0.08704 (9) | 0.0445 (4) |
| C13 | 0.90974 (11) | 0.2583 (2) | -0.05073 (10) | 0.0454 (4) |
| H1 | 0.74570 | 0.78940 | 0.10620 | 0.0690* |

| | | | | |
|------|---------|---------|----------|---------|
| H2 | 0.65710 | 0.70230 | 0.22810 | 0.0800* |
| H3 | 0.55530 | 0.37280 | 0.22100 | 0.0780* |
| H4 | 0.54920 | 0.12080 | 0.09630 | 0.0760* |
| H5 | 0.64400 | 0.19820 | -0.02220 | 0.0670* |
| H11A | 0.91180 | 0.49090 | -0.27460 | 0.0960* |
| H11B | 1.01490 | 0.57240 | -0.18750 | 0.0960* |
| H11C | 0.93350 | 0.74740 | -0.25510 | 0.0960* |
| H14 | 1.01490 | 0.07930 | -0.07260 | 0.0940* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|------------|-------------|
| O9 | 0.0729 (7) | 0.0625 (7) | 0.0640 (7) | 0.0040 (5) | 0.0289 (6) | 0.0164 (5) |
| O14 | 0.0661 (7) | 0.0664 (7) | 0.0657 (7) | 0.0140 (5) | 0.0357 (5) | 0.0054 (5) |
| O15 | 0.0618 (6) | 0.0630 (7) | 0.0569 (6) | 0.0092 (5) | 0.0275 (5) | 0.0080 (5) |
| N8 | 0.0654 (8) | 0.0622 (8) | 0.0683 (8) | 0.0096 (6) | 0.0312 (7) | 0.0138 (6) |
| C1 | 0.0544 (8) | 0.0569 (9) | 0.0676 (9) | -0.0019 (7) | 0.0264 (7) | -0.0099 (7) |
| C2 | 0.0636 (9) | 0.0795 (11) | 0.0660 (10) | 0.0025 (8) | 0.0328 (8) | -0.0163 (8) |
| C3 | 0.0604 (9) | 0.0801 (11) | 0.0630 (9) | 0.0064 (8) | 0.0332 (7) | 0.0068 (8) |
| C4 | 0.0634 (9) | 0.0615 (9) | 0.0722 (10) | -0.0058 (7) | 0.0304 (8) | 0.0056 (8) |
| C5 | 0.0597 (9) | 0.0553 (9) | 0.0559 (8) | -0.0029 (7) | 0.0226 (7) | -0.0044 (7) |
| C6 | 0.0397 (7) | 0.0511 (8) | 0.0488 (7) | 0.0059 (5) | 0.0155 (5) | 0.0022 (6) |
| C7 | 0.0442 (7) | 0.0481 (7) | 0.0483 (7) | -0.0006 (6) | 0.0142 (6) | 0.0001 (6) |
| C10 | 0.0513 (7) | 0.0547 (8) | 0.0459 (7) | -0.0069 (6) | 0.0147 (6) | -0.0019 (6) |
| C11 | 0.0708 (10) | 0.0761 (11) | 0.0535 (9) | -0.0162 (8) | 0.0297 (8) | -0.0023 (7) |
| C12 | 0.0430 (7) | 0.0496 (7) | 0.0425 (7) | -0.0052 (5) | 0.0145 (5) | -0.0040 (5) |
| C13 | 0.0432 (7) | 0.0510 (8) | 0.0449 (7) | -0.0037 (5) | 0.0169 (5) | -0.0059 (6) |

Geometric parameters (Å, °)

| | | | |
|-------------------------|-------------|--------------------------|-------------|
| O9—N8 | 1.4222 (19) | C7—C12 | 1.4363 (19) |
| O9—C10 | 1.3342 (18) | C10—C12 | 1.3649 (19) |
| O14—C13 | 1.2863 (18) | C10—C11 | 1.481 (2) |
| O15—C13 | 1.2488 (17) | C12—C13 | 1.4593 (18) |
| O14—H14 | 0.8200 | C1—H1 | 0.9300 |
| N8—C7 | 1.3057 (18) | C2—H2 | 0.9300 |
| C1—C2 | 1.384 (2) | C3—H3 | 0.9300 |
| C1—C6 | 1.386 (2) | C4—H4 | 0.9300 |
| C2—C3 | 1.375 (3) | C5—H5 | 0.9300 |
| C3—C4 | 1.378 (3) | C11—H11A | 0.9600 |
| C4—C5 | 1.380 (2) | C11—H11B | 0.9600 |
| C5—C6 | 1.389 (2) | C11—H11C | 0.9600 |
| C6—C7 | 1.4813 (19) | | |
| O9...C10 ⁱ | 3.268 (2) | C10...O15 ⁱⁱⁱ | 3.345 (2) |
| O9...C11 ⁱ | 3.351 (2) | C10...C13 ⁱⁱⁱ | 3.566 (2) |
| O14...O15 ⁱⁱ | 2.6252 (18) | C11...O14 | 2.999 (2) |
| O14...C11 | 2.999 (2) | C11...O9 ^{iv} | 3.351 (2) |

| | | | |
|---------------------------|--------------|---------------------------|--------------|
| O15...C11 ⁱⁱⁱ | 3.316 (2) | C11...N8 ^{iv} | 3.427 (2) |
| O15...O14 ⁱⁱ | 2.6252 (18) | C11...O15 ⁱⁱⁱ | 3.316 (2) |
| O15...C13 ⁱⁱ | 3.367 (2) | C12...C13 ⁱⁱⁱ | 3.496 (2) |
| O15...C5 | 3.132 (2) | C13...O15 ⁱⁱ | 3.367 (2) |
| O15...C6 | 3.102 (2) | C13...C10 ⁱⁱⁱ | 3.566 (2) |
| O15...C10 ⁱⁱⁱ | 3.345 (2) | C13...C12 ⁱⁱⁱ | 3.496 (2) |
| O9...H11A ⁱ | 2.6500 | C13...H14 ⁱⁱ | 2.6600 |
| O14...H11B | 2.6800 | H1...N8 | 2.8200 |
| O14...H14 ⁱⁱ | 2.9000 | H11A...O9 ^{iv} | 2.6500 |
| O15...H11B ⁱⁱⁱ | 2.7700 | H11A...N8 ^{iv} | 2.5100 |
| O15...H14 ⁱⁱ | 1.8100 | H11B...O14 | 2.6800 |
| N8...C11 ⁱ | 3.427 (2) | H11B...O15 ⁱⁱⁱ | 2.7700 |
| N8...H1 | 2.8200 | H14...O14 ⁱⁱ | 2.9000 |
| N8...H11A ⁱ | 2.5100 | H14...O15 ⁱⁱ | 1.8100 |
| C5...O15 | 3.132 (2) | H14...C13 ⁱⁱ | 2.6600 |
| C6...O15 | 3.102 (2) | H14...H14 ⁱⁱ | 2.3700 |
| C10...O9 ^{iv} | 3.268 (2) | | |
| | | | |
| N8—O9—C10 | 109.41 (11) | O14—C13—C12 | 116.24 (12) |
| C13—O14—H14 | 109.00 | O15—C13—C12 | 120.20 (12) |
| O9—N8—C7 | 105.56 (12) | O14—C13—O15 | 123.54 (12) |
| C2—C1—C6 | 119.97 (16) | C2—C1—H1 | 120.00 |
| C1—C2—C3 | 120.23 (16) | C6—C1—H1 | 120.00 |
| C2—C3—C4 | 119.98 (16) | C1—C2—H2 | 120.00 |
| C3—C4—C5 | 120.28 (16) | C3—C2—H2 | 120.00 |
| C4—C5—C6 | 120.02 (15) | C2—C3—H3 | 120.00 |
| C1—C6—C7 | 118.88 (12) | C4—C3—H3 | 120.00 |
| C5—C6—C7 | 121.56 (12) | C3—C4—H4 | 120.00 |
| C1—C6—C5 | 119.49 (13) | C5—C4—H4 | 120.00 |
| N8—C7—C6 | 117.63 (12) | C4—C5—H5 | 120.00 |
| N8—C7—C12 | 111.06 (12) | C6—C5—H5 | 120.00 |
| C6—C7—C12 | 131.31 (11) | C10—C11—H11A | 109.00 |
| O9—C10—C11 | 115.59 (12) | C10—C11—H11B | 109.00 |
| O9—C10—C12 | 109.44 (12) | C10—C11—H11C | 110.00 |
| C11—C10—C12 | 134.94 (13) | H11A—C11—H11B | 110.00 |
| C7—C12—C13 | 128.23 (11) | H11A—C11—H11C | 109.00 |
| C10—C12—C13 | 127.03 (12) | H11B—C11—H11C | 109.00 |
| C7—C12—C10 | 104.53 (11) | | |
| | | | |
| C10—O9—N8—C7 | 0.33 (15) | C1—C6—C7—C12 | 124.36 (16) |
| N8—O9—C10—C11 | -178.39 (12) | C5—C6—C7—N8 | 122.44 (15) |
| N8—O9—C10—C12 | -0.04 (15) | N8—C7—C12—C10 | 0.45 (16) |
| O9—N8—C7—C12 | -0.47 (15) | N8—C7—C12—C13 | 175.43 (13) |
| O9—N8—C7—C6 | 178.53 (11) | C6—C7—C12—C10 | -178.37 (14) |
| C2—C1—C6—C5 | -0.1 (2) | C6—C7—C12—C13 | -3.4 (2) |
| C6—C1—C2—C3 | -1.6 (3) | O9—C10—C12—C7 | -0.23 (15) |
| C2—C1—C6—C7 | 176.80 (14) | O9—C10—C12—C13 | -175.28 (12) |
| C1—C2—C3—C4 | 1.7 (3) | C11—C10—C12—C7 | 177.67 (16) |

| | | | |
|--------------|--------------|-----------------|-------------|
| C2—C3—C4—C5 | -0.2 (3) | C11—C10—C12—C13 | 2.6 (3) |
| C3—C4—C5—C6 | -1.5 (3) | C7—C12—C13—O14 | 178.55 (13) |
| C4—C5—C6—C7 | -175.22 (14) | C7—C12—C13—O15 | -3.3 (2) |
| C4—C5—C6—C1 | 1.6 (2) | C10—C12—C13—O14 | -7.5 (2) |
| C1—C6—C7—N8 | -54.40 (19) | C10—C12—C13—O15 | 170.61 (13) |
| C5—C6—C7—C12 | -58.8 (2) | | |

Symmetry codes: (i) $-x+3/2, y+1/2, -z-1/2$; (ii) $-x+2, -y, -z$; (iii) $-x+2, -y+1, -z$; (iv) $-x+3/2, y-1/2, -z-1/2$.

Hydrogen-bond geometry (Å, °)

| <i>D—H...A</i> | <i>D—H</i> | <i>H...A</i> | <i>D...A</i> | <i>D—H...A</i> |
|-----------------------------|------------|--------------|--------------|----------------|
| O14—H14...O15 ⁱⁱ | 0.82 | 1.81 | 2.6252 (18) | 172 |
| C11—H11A...N8 ^{iv} | 0.96 | 2.51 | 3.427 (2) | 159 |

Symmetry codes: (ii) $-x+2, -y, -z$; (iv) $-x+3/2, y-1/2, -z-1/2$.