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# Crystal structures of (*E*)-*N*′-(2-hydroxy-5-methylbenzylidene)isonicotinohydrazide and (*E*)-*N*′-(5-fluoro-2-hydroxybenzylidene)isonicotinohydrazide

**Kittipong Chainok,[a] Sureerat Makmuang[b] and Filip Kielar[b]***

[a]Department of Physics, Faculty of Science and Technology, Thammasat University, Khlong Luang, Pathum Thani, 12120, Thailand, and [b]Department of Chemistry and Center of Excellence in Biomaterials, Faculty of Science, Naresuan University, Muang, Phitsanulok, 65000, Thailand. *Correspondence e-mail: filipk@nu.ac.th

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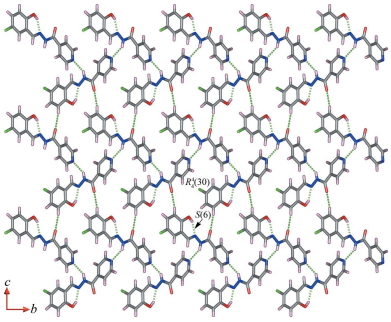
**CCDC references**: 1485834; 1485833

**Supporting information**: this article has supporting information at journals.iucr.org/e

Two derivatives of the well-known iron chelator, (*E*)-*N*′-(2-hydroxybenzylidene)isonicotinohydrazide (SIH), substituted in the 5-position of the 2-hydroxybenzene ring by a methyl and a fluorine group *viz.* (*E*)-*N*′-(2-hydroxy-5-methylbenzylidene)isonicotinohydrazide, $C_{14}H_{13}N_3O_2$, (I), and (*E*)-*N*′-(5-fluoro-2-hydroxybenzylidene)isonicotinohydrazide, $C_{13}H_{10}FN_3O_2$, (II), have been prepared and characterized by single-crystal X-ray diffraction, $^1$H NMR and mass spectrometry. The molecules of both compounds deviate slightly from planarity [r.m.s. deviations are 0.145 and 0.110 Å for (I) and (II), respectively] and adopt an *E* conformation with respect to the double bond of the hydrazone bridge. In each molecule, there is an intramolecular O—H···N hydrogen bond forming an *S*(6) ring motif. The dihedral angles between the mean planes of the isonicotinoyl ring and the cresol ring in (I) or the fluorophenol ring in (II) are 10.49 (6) and 9.43 (6)°, respectively. In the crystals of both compounds, zigzag chains are formed *via* N—H···N hydrogen bonds, in the [10$\bar{1}$] direction for (I) and [010] for (II). In (I), the chains are linked by weak C—H···$\pi$ and $\pi$–$\pi$ stacking interactions [centroid-to-centroid distances = 3.6783 (8) Å; inter-planar angle = 10.94 (5)°], leading to the formation of a three-dimensional supramolecular architecture. In (II), adjacent chains are connected through C—H···O hydrogen bonds to form sheets parallel to (100), which enclose $R_4^4(30)$ ring motifs. The sheets are linked by weak C—H···$\pi$ and $\pi$–$\pi$ [centroid-to-centroid distance = 3.7147 (8) Å; inter-planar angle = 10.94 (5)°] interactions, forming a three-dimensional supramolecular architecture.

## 1. Chemical context

Hydrazone-based chelators for metal ions have received a significant amount of attention (Bendova *et al.*, 2010; Hrušková *et al.*, 2016). Compounds from this class, such as salicyl aldehyde isonicotinoyl hydrazide (SIH), have been studied as potential metal chelators in biological systems (Hrušková *et al.*, 2011). These compounds have also been shown to be effective in protecting against metal-based oxidative stress (Jansová *et al.*, 2014). In our research we are interested in developing probes for metal ions (Carter *et al.*, 2014). We have therefore synthesized the title compounds, which are derivatives of the chelator SIH containing a signalling unit.




## 2. Structural commentary

The molecular structures of the title compounds, (I) and (II), are illustrated in Figs. 1 and 2, respectively. They consist of an

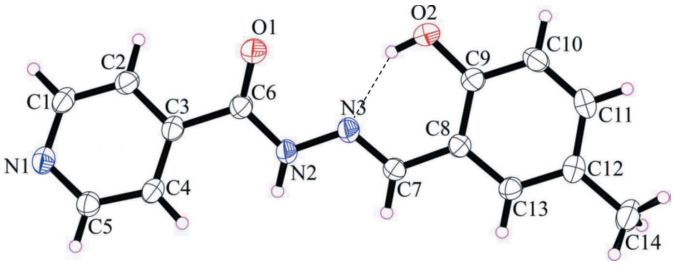



**Figure 1**
The molecular structure of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. The intramolecular O—H···N hydrogen bond is shown as a dashed line (see Table 1).

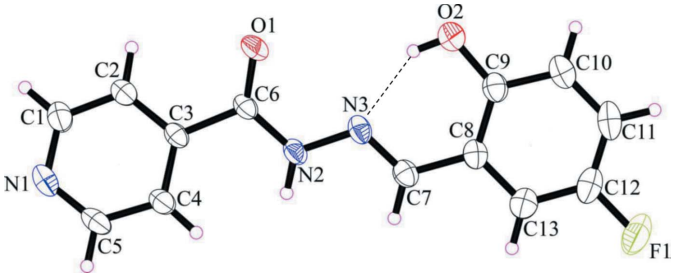
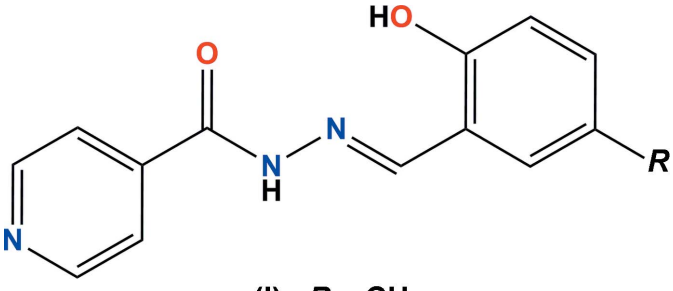



**Figure 2**
The molecular structure of compound (II), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. The intramolecular O—H···N hydrogen bond is shown as a dashed line (see Table 2).

isonicotinoyl moiety linked by a –C7═N3–N2– linkage to a cresol unit in (I) and a fluorophenol ring in (II). The molecules deviate slightly from planarity with the r.m.s deviations for the fitted atoms being 0.145 for (I) and 0.110 Å for (II). In each molecule, there is an intramolecular O—H···N hydrogen bond forming an *S*(6) ring motif. Both compounds have an *E* conformation with respect to the double bond of the hydrazone bridge (C7═N3) with the C8—C7═N3—N2 torsion angles being −179.03 (12) and −177.61 (11)° for (I) and (II), respectively. The dihedral angles between the mean planes of the isonicotinoyl moiety and the cresol moiety in (I), or the fluorophenol moiety in (II) are 10.49 (6) and 9.43 (6)°, respectively. The bond lengths and angles in the title molecules agree reasonably well with those found in closely related structures (Chumakov *et al.*, 2001; Yang, 2006*a*,*b*; Kargar *et al.*, 2010; Sedaghat *et al.*, 2014)




**(I)** $R = CH_3$
**(II)** $R = F$

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

*Cg*1 is the centroid of the N1/C1–C5 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2*O*···N3 | 0.82 | 1.87 | 2.5857 (16) | 145 |
| N2—H2*N*···N1$^{i}$ | 0.86 | 2.19 | 3.0232 (17) | 164 |
| C10—H10···*Cg*1$^{ii}$ | 0.93 | 2.85 | 3.5259 (17) | 130 |

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

**Table 2**
Hydrogen-bond geometry (Å, °) for (II).

*Cg*1 is the centroid of the N1/C1–C5 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2···N3 | 0.82 | 1.92 | 2.6329 (15) | 145 |
| N2—H2*A*···N1$^{i}$ | 0.86 | 2.19 | 2.8889 (15) | 138 |
| C10—H10···O1$^{ii}$ | 0.93 | 2.51 | 3.2573 (18) | 138 |
| C11—H11···*Cg*1$^{iii}$ | 0.93 | 2.98 | 3.8917 (18) | 168 |

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

## 3. Supramolecular features

In the crystals of both compounds, zigzag chains are formed *via* N—H···N hydrogen bonds (Tables 1 and 2), in direction [10$\bar{1}$] for (I) and [010] for (II). In (I), the chains are linked by weak C—H···$\pi$ and $\pi$–$\pi$ stacking interactions [centroid-to-centroid distances = 3.6783 (8) Å; inter-planar angle = 10.94 (5)°], leading to the formation of a three-dimensional supramolecular architecture (Fig. 3). In (II), adjacent chains are connected through C—H···O hydrogen bonds to form sheets parallel to (100), which enclose $R_4^4(30)$ ring motifs. Weak C—H···$\pi$ and $\pi$—$\pi$ [centroid-to-centroid distance = 3.7147 (8) Å, inter-planar angle = 10.94 (5)°] interactions link

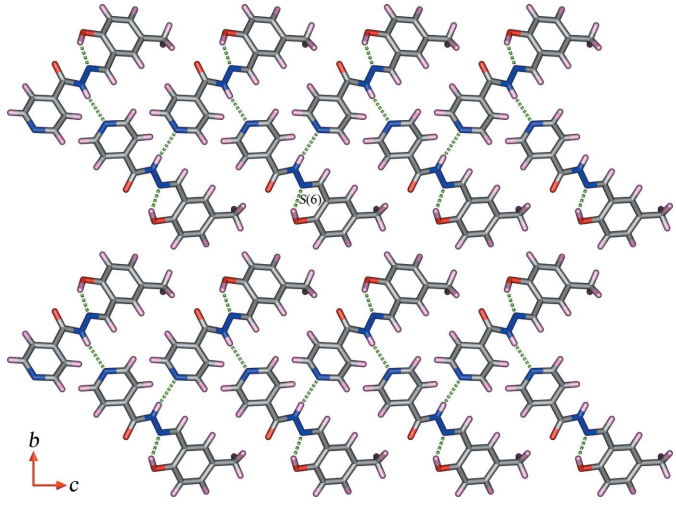



**Figure 3**
Partial view along the *a* axis of the crystal packing of compound (I), showing the hydrogen-bonded (dashed lines; see Table 1) zigzag chains parallel to [10$\bar{1}$].

**Table 3**
Experimental details.

| | (I) | (II) |
|---|---|---|
| Crystal data | | |
| Chemical formula | $C_{14}H_{13}N_3O_2$ | $C_{13}H_{10}FN_3O_2$ |
| $M_r$ | 255.27 | 259.24 |
| Crystal system, space group | Monoclinic, $P2_1/n$ | Monoclinic, $P2_1/c$ |
| Temperature (K) | 296 | 296 |
| $a, b, c$ (Å) | 8.5318 (4), 15.9973 (8), 9.4637 (5) | 8.9195 (3), 10.1128 (3), 13.6254 (4) |
| $\beta$ (°) | 102.738 (2) | 103.481 (1) |
| $V$ (Å$^3$) | 1259.87 (11) | 1195.16 (6) |
| $Z$ | 4 | 4 |
| Radiation type | Mo $K\alpha$ | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.09 | 0.11 |
| Crystal size (mm) | 0.30 × 0.22 × 0.22 | 0.32 × 0.26 × 0.26 |
| Data collection | | |
| Diffractometer | Bruker D8 QUEST CMOS | Bruker APEX2 D8 QUEST CMOS |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2014) | Multi-scan (*SADABS*; Bruker, 2014) |
| $T_{min}$, $T_{max}$ | 0.685, 0.746 | 0.685, 0.746 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 26052, 2996, 2111 | 31833, 2848, 2128 |
| $R_{int}$ | 0.045 | 0.039 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.659 | 0.658 |
| Refinement | | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.046, 0.126, 1.01 | 0.042, 0.124, 1.03 |
| No. of reflections | 2996 | 2848 |
| No. of parameters | 174 | 174 |
| H-atom treatment | H-atom parameters constrained | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.20, −0.22 | 0.26, −0.29 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006), *publCIF* (Westrip, 2010) and *enCIFer* (Allen *et al.*, 2004).

the sheets, forming a three-dimensional supramolecular architecture (Fig. 4).

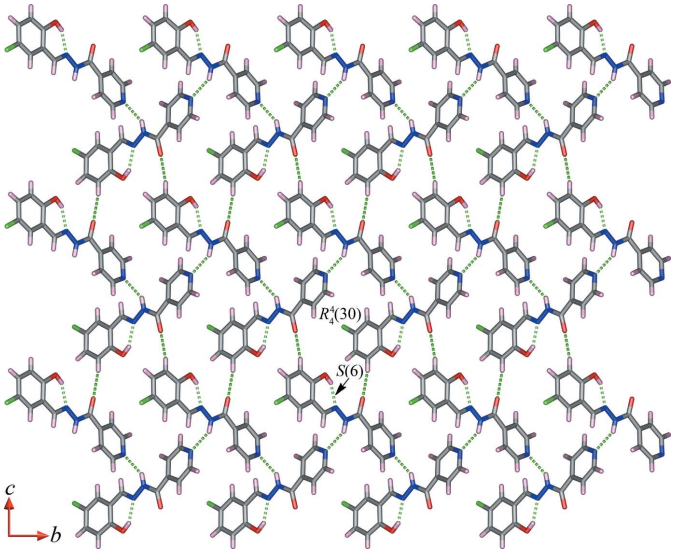



**Figure 4**
Partial view along the *a* axis of the crystal packing of compound (II), showing the N—H···N and C—H···O hydrogen-bonded (dashed lines; see Table 2) sheet propagating in the *bc* plane.

## 4. Database survey

A search of the Cambridge Structural Database (Version 5.37, last update November 2015; Groom *et al.*, 2016) indicated the presence of 40 structures containing the (*E*)-*N*-(2-hydroxybezylydene)isonicotinohydrazide substructure. They include the isotypic crystal structures with chloride (UCAREV, Chumakov *et al.*, 2001; UCAREV01, Yang, 2006*a*), bromide (XENDOK, Yang, 2006*b*; XENDOK01, Sedaghat *et al.*, 2014) and methoxy (VACHAK, Kargar *et al.*, 2010) groups substituted at the 5-position of the phenyl ring. In the crystals of all three compounds, the N—H···N hydrogen bond involving the hydrazone hydrogen and the pyridine nitrogen atoms organize the molecules into a herringbone motif, while in the crystal of the methoxy compound there are also weak N—H···O and C—H···O hydrogen bonds present forming $R_1^2(6)$ ring motifs.

## 5. Synthesis and crystallization

A solution of isonicotinic acid hydrazide (0.184 g, 1.34 mmol) and the appropriately substituted salicyl aldehyde (1.47 mmol) in a mixture of ethanol (3 ml) and water (1 ml) containing a catalytic amount of acetic acid was heated to reflux for 5 h. The reaction mixture was allowed to cool to room temperature, resulting in the formation of a white precipitate. The reaction mixture was filtered and the isolated solid was washed with diethyl ether and dried *in vacuo*. The compounds were isolated as white crystalline solids in 73% and 66% yield for

the methyl (I) and fluoro (II) derivatives, respectively. Single crystals suitable for X-ray diffraction were grown by slow evaporation of methanolic solutions of the title compounds.

Spectroscopic data for (I): $^1$H NMR (400 MHz, DMSO-$d_6$) $d$ 2.25 (1H, $s$, $CH_3$), 6.84 (1H, $d$, $J$ = 8.4, CH—Ph), 7.12 (1H, $dd$, $J$ = 2.0, $J$ = 8.4, CH—Ph), 7.40 (1H, $d$, $J$ = 1.6, CH—Ph), 7.84 (2H, $d$, $J$ = 6.0, CH—Py), 8.63 (1H, $s$, CH═N), 8.79 (2H, $d$, $J$ = 6.0, CH—Py), 10.82 (1H, $s$, NH), 12.26 (1H, $s$, OH). HR–MS (ES$^+$) $C_{14}H_{14}N_3O_2$ requires 256.1086 $[M+H]^+$; found 256.1051.

Spectroscopic data for (II): $^1$H NMR (400 MHz, DMSO-$d_6$) d 6.94 (1H, $dd$, $J$ = 4.4, $J$ = 8.8, CH—Ph), 7.16 (1H, $td$, $J$ = 3.2, $J$ = 8.8, CH—Ph), 7.46 (1H, $dd$, $J$ = 3.2, $J$ = 9.6, CH—Ph), 7.84 (2H, $d$, $J$ = 6.0, CH—Py), 8.67 (1H, $s$, CH═N), 8.80 (2H, $d$, $J$ = 6.0, CH—Py), 10.84 (1H, $s$, NH), 12.35 (1H, $s$, OH). HR–MS (ES$^+$) $C_{13}H_{11}FN_3O_2$ requires 260.0835 $[M+H]^+$; found 260.0831.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms bonded to C, N, and O atoms were placed at calculated positions and refined using a riding-model approximation: N—H = 0.86 Å, O—H = 0.82 Å, and C—H = 0.93–0.96 Å with $U_{iso}$(H) = 1.5$U_{eq}$(C-methyl,O) and 1.2$U_{eq}$(N,C) for other H atoms.

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# supporting information

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# Crystal structures of (*E*)-*N*′-(2-hydroxy-5-methylbenzylidene)isonicotinohydrazide and (*E*)-*N*′-(5-fluoro-2-hydroxybenzylidene)isonicotinohydrazide

**Kittipong Chainok, Sureerat Makmuang and Filip Kielar**

## Computing details

For both compounds, data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009), *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010) and *enCIFer* (Allen *et al.*, 2004).

### (I) (*E*)-*N*′-(2-Hydroxy-5-methylbenzylidene)isonicotinohydrazide

*Crystal data*

$C_{14}H_{13}N_3O_2$
$M_r$ = 255.27
Monoclinic, $P2_1/n$
$a$ = 8.5318 (4) Å
$b$ = 15.9973 (8) Å
$c$ = 9.4637 (5) Å
$\beta$ = 102.738 (2)°
$V$ = 1259.87 (11) Å$^3$
$Z$ = 4
$F(000)$ = 536
$D_x$ = 1.346 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 6456 reflections
$\theta$ = 2.9–27.3°
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 K
Block, colourless
0.30 × 0.22 × 0.22 mm

*Data collection*

Bruker D8 QUEST CMOS diffractometer
Radiation source: microfocus sealed x-ray tube, Incoatec I$\mu$us
GraphiteDouble Bounce Multilayer Mirror monochromator
Detector resolution: 10.5 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
$T_{min}$ = 0.685, $T_{max}$ = 0.746
26052 measured reflections
2996 independent reflections
2111 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.045
$\theta_{max}$ = 27.9°, $\theta_{min}$ = 2.9°
$h$ = −11→11
$k$ = −21→21
$l$ = −12→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.126
$S$ = 1.01
2996 reflections
174 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.2954P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å$^{-3}$
$\Delta\rho_{min} = -0.22$ 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.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.55036 (17) | 0.49610 (7) | 0.82618 (13) | 0.0710 (4) |
| O2 | 0.21987 (15) | 0.36743 (7) | 0.62695 (11) | 0.0575 (3) |
| H2O | 0.2779 | 0.4085 | 0.6481 | 0.086* |
| N1 | 0.84669 (14) | 0.76238 (8) | 0.96854 (13) | 0.0422 (3) |
| N2 | 0.43283 (14) | 0.57825 (7) | 0.63975 (12) | 0.0390 (3) |
| H2N | 0.4281 | 0.6255 | 0.5957 | 0.047* |
| N3 | 0.33377 (14) | 0.51301 (7) | 0.58586 (13) | 0.0392 (3) |
| C1 | 0.81205 (18) | 0.69573 (9) | 1.04127 (15) | 0.0430 (4) |
| H1 | 0.8580 | 0.6923 | 1.1398 | 0.052* |
| C2 | 0.71232 (18) | 0.63196 (9) | 0.97872 (15) | 0.0418 (4) |
| H2 | 0.6922 | 0.5868 | 1.0340 | 0.050* |
| C3 | 0.64217 (16) | 0.63598 (8) | 0.83192 (15) | 0.0362 (3) |
| C4 | 0.67688 (16) | 0.70444 (9) | 0.75506 (15) | 0.0377 (3) |
| H4 | 0.6321 | 0.7096 | 0.6565 | 0.045* |
| C5 | 0.77918 (17) | 0.76509 (9) | 0.82720 (15) | 0.0406 (3) |
| H5 | 0.8025 | 0.8106 | 0.7741 | 0.049* |
| C6 | 0.53873 (18) | 0.56378 (9) | 0.76673 (16) | 0.0415 (3) |
| C7 | 0.23407 (16) | 0.51994 (8) | 0.46483 (14) | 0.0365 (3) |
| H7 | 0.2291 | 0.5691 | 0.4116 | 0.044* |
| C8 | 0.12838 (16) | 0.45084 (8) | 0.41038 (14) | 0.0336 (3) |
| C9 | 0.12462 (17) | 0.37797 (9) | 0.49306 (15) | 0.0393 (3) |
| C10 | 0.02068 (19) | 0.31395 (9) | 0.43625 (17) | 0.0463 (4) |
| H10 | 0.0153 | 0.2664 | 0.4914 | 0.056* |
| C11 | −0.07485 (18) | 0.31991 (10) | 0.29884 (17) | 0.0453 (4) |
| H11 | −0.1419 | 0.2755 | 0.2622 | 0.054* |
| C12 | −0.07365 (16) | 0.39037 (10) | 0.21364 (15) | 0.0409 (4) |
| C13 | 0.02749 (17) | 0.45510 (9) | 0.27258 (15) | 0.0378 (3) |
| H13 | 0.0283 | 0.5034 | 0.2182 | 0.045* |
| C14 | −0.1769 (2) | 0.39481 (12) | 0.06279 (18) | 0.0601 (5) |
| H14A | −0.1905 | 0.3397 | 0.0218 | 0.090* |
| H14B | −0.1260 | 0.4299 | 0.0039 | 0.090* |
| H14C | −0.2800 | 0.4176 | 0.0664 | 0.090* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0903 (10) | 0.0412 (7) | 0.0624 (8) | −0.0114 (6) | −0.0244 (7) | 0.0126 (6) |
| O2 | 0.0751 (8) | 0.0487 (7) | 0.0403 (6) | −0.0108 (6) | −0.0055 (5) | 0.0119 (5) |
| N1 | 0.0409 (7) | 0.0425 (7) | 0.0401 (7) | 0.0010 (5) | 0.0022 (5) | −0.0074 (5) |
| N2 | 0.0408 (7) | 0.0309 (6) | 0.0400 (7) | −0.0020 (5) | −0.0022 (5) | −0.0019 (5) |
| N3 | 0.0409 (7) | 0.0332 (6) | 0.0404 (7) | −0.0023 (5) | 0.0021 (5) | −0.0041 (5) |
| C1 | 0.0457 (8) | 0.0465 (9) | 0.0320 (7) | 0.0056 (7) | −0.0018 (6) | −0.0044 (6) |
| C2 | 0.0475 (8) | 0.0376 (8) | 0.0368 (8) | 0.0037 (6) | 0.0019 (6) | 0.0009 (6) |
| C3 | 0.0341 (7) | 0.0348 (7) | 0.0368 (7) | 0.0065 (6) | 0.0018 (6) | −0.0044 (6) |
| C4 | 0.0371 (8) | 0.0406 (8) | 0.0323 (7) | 0.0043 (6) | 0.0011 (6) | −0.0025 (6) |
| C5 | 0.0419 (8) | 0.0392 (8) | 0.0391 (8) | 0.0003 (6) | 0.0057 (6) | −0.0022 (6) |
| C6 | 0.0446 (8) | 0.0357 (8) | 0.0395 (8) | 0.0018 (6) | −0.0007 (6) | −0.0010 (6) |
| C7 | 0.0411 (8) | 0.0301 (7) | 0.0368 (7) | 0.0008 (6) | 0.0053 (6) | 0.0005 (6) |
| C8 | 0.0354 (7) | 0.0314 (7) | 0.0339 (7) | 0.0027 (6) | 0.0076 (5) | −0.0027 (5) |
| C9 | 0.0439 (8) | 0.0386 (8) | 0.0350 (7) | −0.0010 (6) | 0.0076 (6) | 0.0011 (6) |
| C10 | 0.0547 (9) | 0.0361 (8) | 0.0491 (9) | −0.0080 (7) | 0.0136 (7) | 0.0034 (6) |
| C11 | 0.0411 (8) | 0.0418 (8) | 0.0531 (9) | −0.0100 (7) | 0.0107 (7) | −0.0105 (7) |
| C12 | 0.0348 (7) | 0.0454 (8) | 0.0406 (8) | 0.0022 (6) | 0.0046 (6) | −0.0080 (6) |
| C13 | 0.0408 (8) | 0.0344 (7) | 0.0362 (7) | 0.0032 (6) | 0.0041 (6) | 0.0012 (6) |
| C14 | 0.0527 (10) | 0.0672 (11) | 0.0513 (10) | −0.0003 (9) | −0.0081 (8) | −0.0085 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C6 | 1.2140 (17) | C5—H5 | 0.9300 |
| O2—H2O | 0.8200 | C7—H7 | 0.9300 |
| O2—C9 | 1.3566 (17) | C7—C8 | 1.4476 (19) |
| N1—C1 | 1.3371 (19) | C8—C9 | 1.4083 (19) |
| N1—C5 | 1.3353 (18) | C8—C13 | 1.3969 (18) |
| N2—H2N | 0.8600 | C9—C10 | 1.383 (2) |
| N2—N3 | 1.3687 (16) | C10—H10 | 0.9300 |
| N2—C6 | 1.3547 (17) | C10—C11 | 1.377 (2) |
| N3—C7 | 1.2720 (17) | C11—H11 | 0.9300 |
| C1—H1 | 0.9300 | C11—C12 | 1.387 (2) |
| C1—C2 | 1.376 (2) | C12—C13 | 1.384 (2) |
| C2—H2 | 0.9300 | C12—C14 | 1.505 (2) |
| C2—C3 | 1.3878 (19) | C13—H13 | 0.9300 |
| C3—C4 | 1.382 (2) | C14—H14A | 0.9600 |
| C3—C6 | 1.5011 (19) | C14—H14B | 0.9600 |
| C4—H4 | 0.9300 | C14—H14C | 0.9600 |
| C4—C5 | 1.3808 (19) | | |
| | | | |
| C9—O2—H2O | 109.5 | C8—C7—H7 | 120.2 |
| C5—N1—C1 | 116.49 (12) | C9—C8—C7 | 121.54 (12) |
| N3—N2—H2N | 122.1 | C13—C8—C7 | 120.15 (12) |
| C6—N2—H2N | 122.1 | C13—C8—C9 | 118.31 (12) |
| C6—N2—N3 | 115.88 (12) | O2—C9—C8 | 122.64 (13) |

| | | | |
|---|---|---|---|
| C7—N3—N2 | 120.30 (12) | O2—C9—C10 | 118.14 (13) |
| N1—C1—H1 | 118.1 | C10—C9—C8 | 119.21 (13) |
| N1—C1—C2 | 123.76 (13) | C9—C10—H10 | 119.6 |
| C2—C1—H1 | 118.1 | C11—C10—C9 | 120.72 (14) |
| C1—C2—H2 | 120.5 | C11—C10—H10 | 119.6 |
| C1—C2—C3 | 119.05 (14) | C10—C11—H11 | 119.1 |
| C3—C2—H2 | 120.5 | C10—C11—C12 | 121.76 (13) |
| C2—C3—C6 | 117.42 (13) | C12—C11—H11 | 119.1 |
| C4—C3—C2 | 117.92 (13) | C11—C12—C14 | 120.79 (14) |
| C4—C3—C6 | 124.62 (12) | C13—C12—C11 | 117.23 (13) |
| C3—C4—H4 | 120.6 | C13—C12—C14 | 121.98 (15) |
| C5—C4—C3 | 118.81 (13) | C8—C13—H13 | 118.6 |
| C5—C4—H4 | 120.6 | C12—C13—C8 | 122.74 (13) |
| N1—C5—C4 | 123.95 (14) | C12—C13—H13 | 118.6 |
| N1—C5—H5 | 118.0 | C12—C14—H14A | 109.5 |
| C4—C5—H5 | 118.0 | C12—C14—H14B | 109.5 |
| O1—C6—N2 | 122.27 (13) | C12—C14—H14C | 109.5 |
| O1—C6—C3 | 121.01 (13) | H14A—C14—H14B | 109.5 |
| N2—C6—C3 | 116.73 (12) | H14A—C14—H14C | 109.5 |
| N3—C7—H7 | 120.2 | H14B—C14—H14C | 109.5 |
| N3—C7—C8 | 119.63 (13) | | |

| | | | |
|---|---|---|---|
| O2—C9—C10—C11 | −177.73 (14) | C5—N1—C1—C2 | −0.3 (2) |
| N1—C1—C2—C3 | −0.2 (2) | C6—N2—N3—C7 | −177.70 (13) |
| N2—N3—C7—C8 | −179.03 (12) | C6—C3—C4—C5 | −177.39 (13) |
| N3—N2—C6—O1 | 3.1 (2) | C7—C8—C9—O2 | −0.7 (2) |
| N3—N2—C6—C3 | −176.69 (12) | C7—C8—C9—C10 | 179.63 (13) |
| N3—C7—C8—C9 | 4.8 (2) | C7—C8—C13—C12 | 178.65 (13) |
| N3—C7—C8—C13 | −174.87 (13) | C8—C7—N3—N2 | −179.03 (12) |
| C1—N1—C5—C4 | 0.7 (2) | C8—C9—C10—C11 | 1.9 (2) |
| C1—C2—C3—C4 | 0.2 (2) | C9—C8—C13—C12 | −1.0 (2) |
| C1—C2—C3—C6 | 177.94 (13) | C9—C10—C11—C12 | −1.5 (2) |
| C2—C3—C4—C5 | 0.1 (2) | C10—C11—C12—C13 | −0.2 (2) |
| C2—C3—C6—O1 | −19.9 (2) | C10—C11—C12—C14 | 178.89 (15) |
| C2—C3—C6—N2 | 159.99 (13) | C11—C12—C13—C8 | 1.5 (2) |
| C3—C4—C5—N1 | −0.6 (2) | C13—C8—C9—O2 | 178.91 (14) |
| C4—C3—C6—O1 | 157.69 (16) | C13—C8—C9—C10 | −0.7 (2) |
| C4—C3—C6—N2 | −22.5 (2) | C14—C12—C13—C8 | −177.64 (14) |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the N1/C1–C5 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2*O*···N3 | 0.82 | 1.87 | 2.5857 (16) | 145 |
| N2—H2*N*···N1$^{i}$ | 0.86 | 2.19 | 3.0232 (17) | 164 |
| C10—H10···*Cg*1$^{ii}$ | 0.93 | 2.85 | 3.5259 (17) | 130 |

Symmetry codes: (i) *x*−1/2, −*y*+3/2, *z*−1/2; (ii) −*x*+1/2, *y*−1/2, −*z*+3/2.

**(II) (*E*)-*N*′-(5-Fluoro-2-hydroxybenzylidene)isonicotinohydrazide**

*Crystal data*

$C_{13}H_{10}FN_3O_2$
$M_r = 259.24$
Monoclinic, $P2_1/c$
$a = 8.9195$ (3) Å
$b = 10.1128$ (3) Å
$c = 13.6254$ (4) Å
$\beta = 103.481$ (1)°
$V = 1195.16$ (6) Å$^3$
$Z = 4$
$F(000) = 536$
$D_x = 1.441$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9934 reflections
$\theta = 3.1$–$28.5$°
$\mu = 0.11$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.32 × 0.26 × 0.26 mm

*Data collection*

Bruker APEX2 D8 QUEST CMOS diffractometer
Radiation source: microfocus sealed x-ray tube, Incoatec I$\mu$us
GraphiteDouble Bounce Multilayer Mirror monochromator
Detector resolution: 10.5 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
$T_{min} = 0.685$, $T_{max} = 0.746$
31833 measured reflections
2848 independent reflections
2128 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.9°$, $\theta_{min} = 3.1°$
$h = -11 \rightarrow 11$
$k = -13 \rightarrow 13$
$l = -17 \rightarrow 17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.124$
$S = 1.03$
2848 reflections
174 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2 + 0.282P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å$^{-3}$
$\Delta\rho_{min} = -0.29$ e Å$^{-3}$
Extinction correction: SHELXL2014 (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.020 (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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F1 | 0.20524 (13) | −0.04313 (11) | 0.46463 (10) | 0.0868 (4) |
| O1 | 0.82356 (13) | 0.59703 (11) | 0.44402 (7) | 0.0572 (3) |
| O2 | 0.53778 (15) | 0.31773 (13) | 0.30688 (8) | 0.0650 (3) |
| H2 | 0.5959 | 0.3608 | 0.3508 | 0.097* |
| N1 | 1.11088 (14) | 0.82083 (13) | 0.75798 (9) | 0.0497 (3) |
| N2 | 0.75299 (13) | 0.47336 (11) | 0.56431 (8) | 0.0404 (3) |

| | | | | |
|---|---|---|---|---|
| H2A | 0.7633 | 0.4582 | 0.6276 | 0.048* |
| N3 | 0.65442 (13) | 0.39828 (11) | 0.49277 (8) | 0.0410 (3) |
| C1 | 1.12858 (18) | 0.81537 (17) | 0.66408 (12) | 0.0553 (4) |
| H1 | 1.2031 | 0.8689 | 0.6466 | 0.066* |
| C2 | 1.04204 (17) | 0.73427 (16) | 0.59110 (11) | 0.0497 (4) |
| H2B | 1.0577 | 0.7346 | 0.5260 | 0.060* |
| C3 | 0.93237 (14) | 0.65288 (12) | 0.61510 (9) | 0.0355 (3) |
| C4 | 0.91374 (17) | 0.65656 (14) | 0.71277 (10) | 0.0429 (3) |
| H4 | 0.8417 | 0.6026 | 0.7327 | 0.052* |
| C5 | 1.00507 (19) | 0.74261 (15) | 0.78056 (10) | 0.0502 (4) |
| H5 | 0.9910 | 0.7455 | 0.8460 | 0.060* |
| C6 | 0.83297 (15) | 0.57142 (13) | 0.53241 (9) | 0.0376 (3) |
| C7 | 0.57486 (15) | 0.31041 (13) | 0.52504 (10) | 0.0413 (3) |
| H7 | 0.5825 | 0.3020 | 0.5940 | 0.050* |
| C8 | 0.47255 (15) | 0.22351 (13) | 0.45483 (10) | 0.0408 (3) |
| C9 | 0.46263 (16) | 0.22688 (15) | 0.35051 (11) | 0.0457 (3) |
| C10 | 0.37199 (18) | 0.13466 (17) | 0.28799 (13) | 0.0569 (4) |
| H10 | 0.3694 | 0.1346 | 0.2194 | 0.068* |
| C11 | 0.28665 (18) | 0.04408 (16) | 0.32564 (14) | 0.0597 (4) |
| H11 | 0.2260 | −0.0174 | 0.2834 | 0.072* |
| C12 | 0.29224 (18) | 0.04568 (15) | 0.42667 (15) | 0.0567 (4) |
| C13 | 0.38397 (17) | 0.13144 (15) | 0.49236 (12) | 0.0499 (4) |
| H13 | 0.3870 | 0.1282 | 0.5610 | 0.060* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.0769 (7) | 0.0678 (7) | 0.1118 (9) | −0.0293 (6) | 0.0143 (7) | 0.0139 (6) |
| O1 | 0.0767 (7) | 0.0616 (7) | 0.0271 (5) | −0.0163 (6) | −0.0006 (5) | −0.0004 (4) |
| O2 | 0.0697 (8) | 0.0754 (8) | 0.0453 (6) | −0.0252 (6) | 0.0041 (5) | −0.0007 (6) |
| N1 | 0.0495 (7) | 0.0494 (7) | 0.0426 (7) | 0.0033 (6) | −0.0048 (5) | −0.0125 (5) |
| N2 | 0.0452 (6) | 0.0399 (6) | 0.0297 (5) | −0.0020 (5) | −0.0040 (4) | −0.0007 (4) |
| N3 | 0.0404 (6) | 0.0380 (6) | 0.0379 (6) | 0.0007 (5) | −0.0044 (5) | −0.0031 (5) |
| C1 | 0.0519 (9) | 0.0616 (10) | 0.0502 (9) | −0.0136 (8) | 0.0077 (7) | −0.0123 (7) |
| C2 | 0.0530 (8) | 0.0598 (9) | 0.0356 (7) | −0.0099 (7) | 0.0092 (6) | −0.0088 (6) |
| C3 | 0.0382 (7) | 0.0351 (6) | 0.0291 (6) | 0.0058 (5) | −0.0007 (5) | −0.0021 (5) |
| C4 | 0.0532 (8) | 0.0409 (7) | 0.0324 (6) | 0.0015 (6) | 0.0051 (6) | −0.0022 (5) |
| C5 | 0.0662 (9) | 0.0509 (8) | 0.0294 (6) | 0.0075 (8) | 0.0026 (6) | −0.0066 (6) |
| C6 | 0.0418 (7) | 0.0377 (7) | 0.0285 (6) | 0.0027 (6) | −0.0011 (5) | −0.0016 (5) |
| C7 | 0.0413 (7) | 0.0394 (7) | 0.0393 (7) | 0.0042 (6) | 0.0013 (6) | −0.0011 (6) |
| C8 | 0.0348 (7) | 0.0358 (7) | 0.0475 (7) | 0.0039 (5) | 0.0008 (5) | −0.0004 (6) |
| C9 | 0.0396 (7) | 0.0462 (8) | 0.0469 (8) | −0.0005 (6) | 0.0016 (6) | −0.0020 (6) |
| C10 | 0.0514 (9) | 0.0605 (10) | 0.0525 (9) | −0.0037 (8) | −0.0006 (7) | −0.0119 (7) |
| C11 | 0.0464 (8) | 0.0472 (9) | 0.0759 (12) | −0.0042 (7) | −0.0051 (8) | −0.0132 (8) |
| C12 | 0.0435 (8) | 0.0398 (8) | 0.0824 (12) | −0.0038 (6) | 0.0060 (8) | 0.0060 (7) |
| C13 | 0.0452 (8) | 0.0445 (8) | 0.0572 (9) | 0.0022 (6) | 0.0060 (7) | 0.0051 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| F1—C12 | 1.3651 (19) | C3—C6 | 1.5061 (17) |
| O1—C6 | 1.2154 (15) | C4—H4 | 0.9300 |
| O2—H2 | 0.8200 | C4—C5 | 1.387 (2) |
| O2—C9 | 1.3537 (18) | C5—H5 | 0.9300 |
| N1—C1 | 1.3263 (19) | C7—H7 | 0.9300 |
| N1—C5 | 1.322 (2) | C7—C8 | 1.4537 (18) |
| N2—H2A | 0.8600 | C8—C9 | 1.404 (2) |
| N2—N3 | 1.3783 (15) | C8—C13 | 1.393 (2) |
| N2—C6 | 1.3513 (17) | C9—C10 | 1.388 (2) |
| N3—C7 | 1.2775 (18) | C10—H10 | 0.9300 |
| C1—H1 | 0.9300 | C10—C11 | 1.365 (2) |
| C1—C2 | 1.378 (2) | C11—H11 | 0.9300 |
| C2—H2B | 0.9300 | C11—C12 | 1.366 (2) |
| C2—C3 | 1.375 (2) | C12—C13 | 1.372 (2) |
| C3—C4 | 1.3796 (18) | C13—H13 | 0.9300 |
| | | | |
| C9—O2—H2 | 109.5 | N2—C6—C3 | 115.07 (11) |
| C5—N1—C1 | 116.85 (12) | N3—C7—H7 | 119.7 |
| N3—N2—H2A | 120.8 | N3—C7—C8 | 120.53 (13) |
| C6—N2—H2A | 120.8 | C8—C7—H7 | 119.7 |
| C6—N2—N3 | 118.31 (11) | C9—C8—C7 | 122.23 (13) |
| C7—N3—N2 | 116.98 (11) | C13—C8—C7 | 119.03 (13) |
| N1—C1—H1 | 118.4 | C13—C8—C9 | 118.72 (13) |
| N1—C1—C2 | 123.25 (15) | O2—C9—C8 | 122.70 (13) |
| C2—C1—H1 | 118.4 | O2—C9—C10 | 117.61 (14) |
| C1—C2—H2B | 120.2 | C10—C9—C8 | 119.68 (14) |
| C3—C2—C1 | 119.64 (13) | C9—C10—H10 | 119.5 |
| C3—C2—H2B | 120.2 | C11—C10—C9 | 121.06 (15) |
| C2—C3—C4 | 117.76 (12) | C11—C10—H10 | 119.5 |
| C2—C3—C6 | 118.48 (11) | C10—C11—H11 | 120.7 |
| C4—C3—C6 | 123.65 (12) | C10—C11—C12 | 118.57 (14) |
| C3—C4—H4 | 120.8 | C12—C11—H11 | 120.7 |
| C3—C4—C5 | 118.37 (14) | F1—C12—C11 | 118.92 (15) |
| C5—C4—H4 | 120.8 | F1—C12—C13 | 118.30 (16) |
| N1—C5—C4 | 124.13 (13) | C11—C12—C13 | 122.77 (15) |
| N1—C5—H5 | 117.9 | C8—C13—H13 | 120.5 |
| C4—C5—H5 | 117.9 | C12—C13—C8 | 119.09 (15) |
| O1—C6—N2 | 123.74 (12) | C12—C13—H13 | 120.5 |
| O1—C6—C3 | 121.15 (12) | | |
| | | | |
| F1—C12—C13—C8 | −179.45 (13) | C4—C3—C6—N2 | −18.13 (18) |
| O2—C9—C10—C11 | −176.72 (15) | C5—N1—C1—C2 | 0.6 (2) |
| N1—C1—C2—C3 | −0.8 (3) | C6—N2—N3—C7 | −176.78 (12) |
| N2—N3—C7—C8 | −177.61 (11) | C6—C3—C4—C5 | −175.40 (12) |
| N3—N2—C6—O1 | −0.3 (2) | C7—C8—C9—O2 | −5.4 (2) |
| N3—N2—C6—C3 | 177.26 (10) | C7—C8—C9—C10 | 174.98 (13) |

| | | | |
|---|---|---|---|
| N3—C7—C8—C9 | 3.5 (2) | C7—C8—C13—C12 | −177.30 (13) |
| N3—C7—C8—C13 | −178.08 (12) | C8—C7—N3—N2 | −177.61 (11) |
| C1—N1—C5—C4 | 0.2 (2) | C8—C9—C10—C11 | 2.9 (2) |
| C1—C2—C3—C4 | 0.1 (2) | C9—C8—C13—C12 | 1.1 (2) |
| C1—C2—C3—C6 | 176.36 (13) | C9—C10—C11—C12 | −0.1 (2) |
| C2—C3—C4—C5 | 0.6 (2) | C10—C11—C12—F1 | 178.91 (14) |
| C2—C3—C6—O1 | −16.5 (2) | C10—C11—C12—C13 | −2.3 (2) |
| C2—C3—C6—N2 | 165.85 (12) | C11—C12—C13—C8 | 1.7 (2) |
| C3—C4—C5—N1 | −0.8 (2) | C13—C8—C9—O2 | 176.21 (13) |
| C4—C3—C6—O1 | 159.53 (14) | C13—C8—C9—C10 | −3.4 (2) |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the N1/C1–C5 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2···N3 | 0.82 | 1.92 | 2.6329 (15) | 145 |
| N2—H2*A*···N1$^{i}$ | 0.86 | 2.19 | 2.8889 (15) | 138 |
| C10—H10···O1$^{ii}$ | 0.93 | 2.51 | 3.2573 (18) | 138 |
| C11—H11···*Cg*1$^{iii}$ | 0.93 | 2.98 | 3.8917 (18) | 168 |

Symmetry codes: (i) −*x*+2, *y*−1/2, −*z*+3/2; (ii) −*x*+1, *y*−1/2, −*z*+1/2; (iii) *x*−1, −*y*+1/2, *z*−1/2.