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Synthesis, crystal structure and Hirshfeld surface analysis of ethyl (*E*)-2-cyano-3-[5-(4-ethylphenyl)-isoxazol-3-yl]prop-2-enoate

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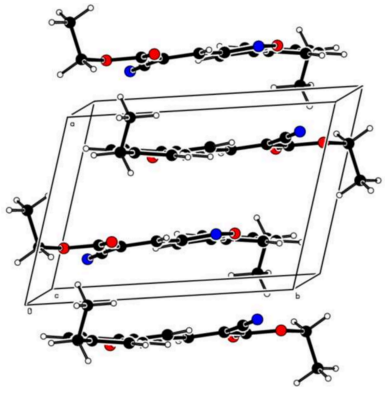
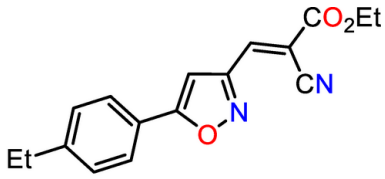
In the molecule of the title compound, $C_{17}H_{16}N_2O_3$, the isoxazol and phenyl rings are oriented at a dihedral angle of 14.84 (5)°. The 2-cyanoacrylate moiety is in *E*- configuration. In the crystal, there are no intermolecular hydrogen-bonding or C—H···π(ring) interactions, only a π–π interaction between the parallel isoxazol rings with centroid-to-centroid distance of 3.4932 (9) Å (α = 0.02°). The Hirshfeld surface analysis indicates that the most important contributions to the crystal packing are from H···H (43.9%), H···N/N···H (17.0%), H···O/O···H (13.9%) and C···C (10.1%) interactions.

1. Chemical context

Esters of cyanoacrylic acid – cyanoacrylates – are well-known to be the components of adhesive compositions. They are also convenient and versatile building blocks in organic synthesis that are widely used in processes of carbon skeleton growth (Ammida & Giath, 2003; Kim *et al.*, 2005; Motokura *et al.*, 2019). They have found wide applications in the syntheses of cyclic and heterocyclic structures, including condensed derivatives. In particular, they are used to obtain polysubstituted cyclopropanes (Zhang *et al.*, 2017), cyclohexenes (Xiao *et al.*, 2012), cyanoanilines (Sharanin *et al.*, 1980), chromenes (Dong *et al.*, 2010; Chang *et al.*, 2021), pyranocoumarines (Xie *et al.*, 2022), pyrrolidines (Imagawa *et al.*, 2016), tetrahydrofurans (Khan *et al.*, 2014), pyrimidines (Moirangthem & Laitonjam, 2009; Sheibani *et al.*, 2009), piperidines (Dong *et al.*, 2021) and others. The most commonly used substrates are 3-aryl and 3-hetaryl 2-cyanoacrylates. As a result of the asymmetry of the spatial structure of the molecule, they can exist in the form of *Z*- and *E*-isomers, which can ultimately affect the spatial structure of the products resulting from the reactions with their participation. The configuration of the trisubstituted double bond of cyanoacrylates depends on the synthesis conditions and structure of the substrates (Irfan *et al.*, 2021). This determines the importance of accurately establishing the crystal structure of cyanoacrylates. Herein, we report on the crystal structure of ethyl (*E*)-2-cyano-3-[5-(4-ethylphenyl)-isoxazol-3-yl]prop-2-enoate (**1**), which we studied as a starting



compound for the synthesis of isoxazole-containing pyrans and chromenes (Potkin *et al.*, 2024). According to literature data, similar in structure aryl and hetaryl cyanoacrylates also have the *E*-configuration of the exocyclic double bond (Deshpande *et al.*, 2012; Franconetti *et al.*, 2016; Kalkhambkar *et al.*, 2012).



2. Structural commentary

The asymmetric unit of the title compound, $C_{17}H_{16}N_2O_3$, contains isoxazol (O1/N2/C3–C5) and phenyl (C11–C16) rings oriented at a dihedral angle of 14.84 (5)° (Fig. 1). The corresponding dihedral angles are reported to be 46.22 (4)° in $C_{17}H_{13}NO_3$ (Benouatas *et al.*, 2021) and 5.50 (8)° in $C_{17}H_{13}NO_2$ (Asiri *et al.*, 2012). Atoms C1, C6, C7, N1 and C17 are located 0.0178 (18), 0.0389 (15), 0.0641 (15), −0.044 (2) and −0.0429 (15) Å, respectively, away from the corresponding ring planes. In the ethyl 2-cyanoacrylate moiety, the C9—O3—C8—C7, O3—C8—C7—C6, C8—C7—C6—C3 and C7—C6—C3—N2 torsion angles are −179.66 (12), 175.16 (13), −177.75 (12) and 179.15 (14)°, respectively, showing an *E*-configuration. Bond lengths and angles agree well with the values observed for the related compounds (*Z*)-4-(2-methoxybenzylidene)-3-phenylisoxazol-5(4*H*)-one (Benouatas *et al.*, 2021) and (4*Z*)-4-benzylidene-2-phenyl-1,3-oxazol-5(*4*H)-one (Asiri *et al.*, 2012).

3. Supramolecular features

In the crystal, the molecules are stacked along the *a*-axis direction (Fig. 2) and there are no intermolecular hydrogen-bonding or C—H···π(ring) interactions, only a π–π interaction between the parallel isoxazol (O1/N2/C3–C5) rings with a centroid-to-centroid distance of 3.4932 (9) Å (α = 0.02°).

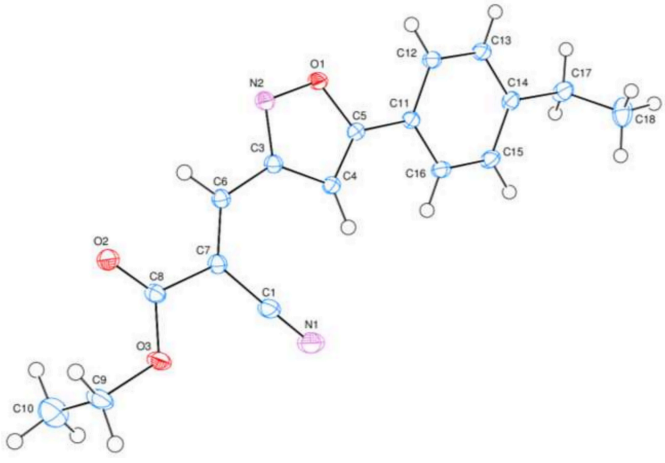


Figure 1
The asymmetric unit of the title compound with atom-numbering scheme and 50% probability ellipsoids.

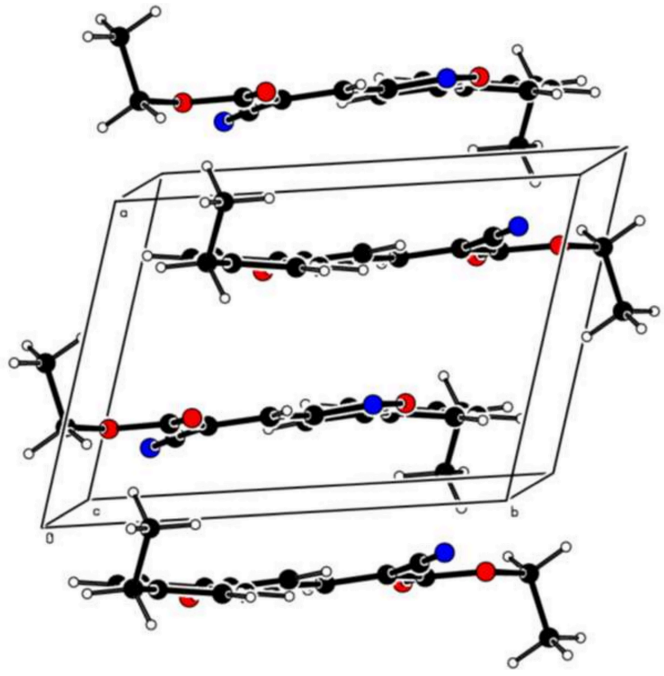


Figure 2
A partial packing diagram for the title compound viewed down the *c*-axis direction.

4. Hirshfeld surface analysis

To visualize the intermolecular interactions in the crystal of title compound, a Hirshfeld surface (HS) analysis was carried out using *Crystal Explorer 17.5* (Spackman *et al.*, 2021). In the HS plotted over d_{norm} (Fig. 3), the white surface indicates contacts with distances equal to the sum of van der Waals radii, and the red and blue colours indicate distances shorter (in close contact) or longer (distinct contact) than the van der Waals radii, respectively (Table 1) (Venkatesan *et al.*, 2016). The appearing bright-red spots indicate their roles as the respective donors and/or acceptors. The shape-index surface can be used to identify characteristic packing modes, in

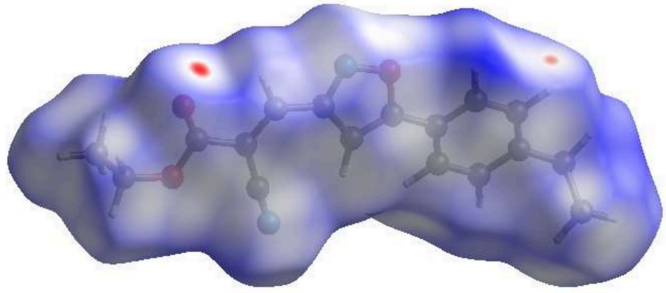


Figure 3
View of the three-dimensional Hirshfeld surface plotted over d_{norm}.

Table 1
Selected interatomic distances (Å).

O1···H12	2.52	C1···C4	3.069 (2)
O1···H9*A*^{i}	2.66	C3···C11^{iv}	3.403 (2)
O2···H9*B*	2.38	C6···C11^{iv}	3.385 (2)
O2···H15^{ii}	2.61	C6···C16^{iv}	3.404 (2)
O2···H6	2.48	C1···H4	2.63
N1···H13^{iii}	2.65	C4···H16	2.82
N1···H4	2.65	H13···H17*A*	2.37
N2···H9*A*^{i}	2.69		

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

particular, planar stacking arrangements and the presence of aromatic stacking interactions such as C—H···π and π–π interactions with the former represented as red π-holes, which are related to the electron ring interactions between the C–H groups with the centroid of the aromatic rings of neighbouring molecules. Fig. 4 clearly suggests that there are no C—H···π interactions. π–π stacking is indicated by the presence of adjacent red and blue triangles; if there are no adjacent red and/or blue triangles, then there are no π–π interactions. Fig. 4 clearly suggests that there are π···π interactions in the title compound. According to the two-dimensional fingerprint plots (Fig. 5), H···H (43.9%), H···N/N···H (17.0%), H···O/O···H (13.9%) and C···C (10.1%) contacts make the most important contributions to the HS.

5. Synthesis and crystallization

Compound **1** was obtained according to the method (Fig. 6) described by us earlier (Potkin *et al.*, 2024). 5-(4-Ethylphenyl) isoxazole-3-carbaldehyde (**2**) (0.50 g, 2.5 mmol) and ethyl cyanoacetate (0.34 g, 3.0 mmol) were dissolved in EtOH (10 ml), 2 drops of piperidine were added and the resulting mixture was stirred for 5 h at 323 K then kept at 278 K overnight. The resulting precipitate was filtered, washed with cold EtOH (2 × 5 ml) and dried under reduced pressure. The obtained product did not require further purification. It was crystallized from methanol solution to give pale creamy needles, yield 0.50 g (67%), m.p. 274–276 K. IR (KBr), ν (cm^{-1}): 2232 (CN), 1737 (C=O), 1663, 1613, 1592, 1561 (1,2-oxazole), 1245 (aromatic C–H), 797 (vinylene –CH=), 534 (–CH=C—CN). ^{1}H NMR ($CDCl_3$, 500 MHz, 301 K): δ = 7.95 (*s*, 1H, –CH=), 7.75 (*d*, 2H, HAr, J = 8.4), 7.37 (*s*, 1H, H4), 7.32 (*d*, 2H, H Ar, J = 8.4), 4.42 (*q*, 2H, CH_2, J = 7.1), 2.71 (*q*, 2H, CH_2, J = 7.6), 1.41 (*t*, 3H, CH_3, J = 7.1), 1.27 (*t*, 3H, CH_3, J = 7.6). ^{13}C NMR ($CDCl_3$, 125 MHz, 301 K): δ = 172.6, 161.0, 157.9, 147.9, 142.8, 128.8 (2C), 124.0, 114.2, 109.8, 97.6, 63.5, 29.0, 15.4, 14.2. MS (APCI): m/z = 296 $[M]^+$ (100).

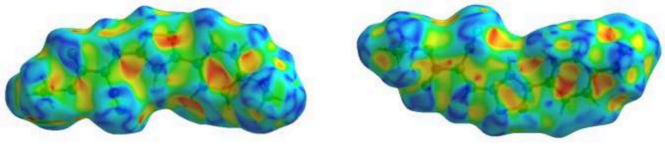


Figure 4
The shape-index surface showing two orientations.

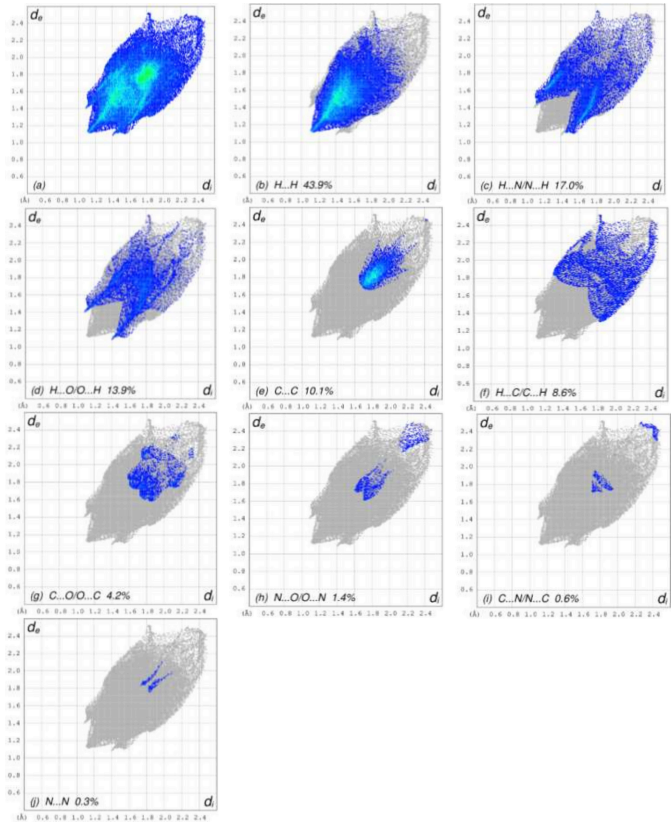


Figure 5
The full two-dimensional fingerprint plots showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) H···N/N···H, (*d*) H···O/O···H, (*e*) C···C, (*f*) H···C/C···H, (*g*) C···O/O···C, (*h*) N···O/O···N, (*i*) C···N/N···C and (*j*) N···N interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound hydrogen-atom positions were calculated geometrically at distances of 0.95 Å (for aromatic CH), 0.99 Å (for CH_2) and 0.98 Å (for CH_3), and refined using a riding model applying the constraint U_{iso} = $k \times U_{eq}$ (C), where k = 1.5 for methyl hydrogens and k = 1.2 for all other hydrogen atoms.

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The authors' contributions are as follows. Conceptualization, TH and MHAD; synthesis, IAK and APSP; NMR analysis, MSG and KIH; X-ray analysis, MSG and NAG; Hirshfeld

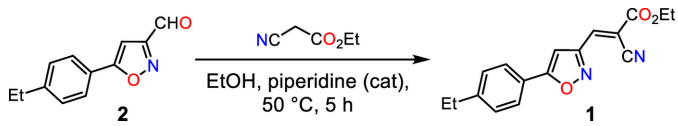

Figure 6
Reaction scheme.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{16}N_2O_3$
M_r	296.32
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	7.2361 (6), 10.1537 (8), 11.1493 (8)
α, β, γ (°)	73.098 (2), 76.611 (3), 72.555 (3)
V (Å^3)	738.32 (10)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.40 × 0.32 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII
Absorption correction	Multi-scan (*SADABS*; Krause et al., 2015)
T_{min}, T_{max}	0.930, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13453, 4283, 3544
R_{int}	0.020
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.703
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.150, 1.02
No. of reflections	4283
No. of parameters	201
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.74, −0.62

Computer programs: *APEX3* and *SAINT* (Bruker, 2014), *SHELXT2019/1* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *SHELXTL* (Sheldrick, 2008).

surface analysis, TH; writing (review and editing of the manuscript), TH and MHAD; funding acquisition, KIH, NAG and TAJ; supervision, TH and MHAD.

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Computing details

Ethyl (*E*)-2-cyano-3-[5-(4-ethylphenyl)isoxazol-3-yl]prop-2-enoate

Crystal data

$C_{17}H_{16}N_2O_3$
$M_r = 296.32$
Triclinic, $P\overline{1}$
$a = 7.2361$ (6) Å
$b = 10.1537$ (8) Å
$c = 11.1493$ (8) Å
$\alpha = 73.098$ (2)°
$\beta = 76.611$ (3)°
$\gamma = 72.555$ (3)°
$V = 738.32$ (10) Å^3
$Z = 2$
$F(000) = 312$
$D_x = 1.333$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5551 reflections
$\theta = 2.5$–30.1°
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Bulk, colourless
0.40 × 0.32 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause et al., 2015)
$T_{min} = 0.930$, $T_{max} = 1.000$
13453 measured reflections
4283 independent reflections
3544 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 30.0°$, $\theta_{min} = 3.8°$
$h = -8 \rightarrow 10$
$k = -14 \rightarrow 14$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.150$
$S = 1.02$
4283 reflections
201 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 0.5251P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.74$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ 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	0.28675 (16)	0.69298 (11)	0.44138 (9)	0.0194 (2)
O2	0.30302 (17)	0.26261 (11)	0.13160 (10)	0.0219 (2)
O3	0.27135 (18)	0.07239 (11)	0.29464 (10)	0.0234 (2)
N1	0.1827 (3)	0.14647 (16)	0.57881 (14)	0.0370 (4)
N2	0.2963 (2)	0.63165 (13)	0.34260 (11)	0.0200 (3)
C1	0.2185 (2)	0.20516 (16)	0.47481 (14)	0.0229 (3)
C3	0.26948 (19)	0.50293 (14)	0.39795 (13)	0.0152 (3)
C4	0.24135 (19)	0.47687 (14)	0.53287 (13)	0.0154 (3)
H4	0.219017	0.393425	0.593852	0.018*
C5	0.25385 (19)	0.59890 (14)	0.55416 (13)	0.0148 (3)
C6	0.27883 (19)	0.41529 (14)	0.31311 (13)	0.0156 (3)
H6	0.301540	0.457438	0.224765	0.019*
C7	0.2590 (2)	0.28166 (14)	0.34550 (13)	0.0159 (3)
C8	0.2809 (2)	0.20658 (14)	0.24319 (13)	0.0166 (3)
C9	0.2914 (3)	−0.01480 (16)	0.20686 (16)	0.0273 (3)
H9A	0.212681	−0.085624	0.245866	0.033*
H9B	0.241248	0.046024	0.128222	0.033*
C10	0.4965 (3)	−0.0876 (2)	0.1760 (2)	0.0374 (4)
H10A	0.572276	−0.017378	0.130783	0.056*
H10B	0.507173	−0.151209	0.121968	0.056*
H10C	0.548105	−0.143216	0.254400	0.056*
C11	0.24115 (19)	0.64417 (14)	0.66934 (12)	0.0147 (3)
C12	0.2177 (2)	0.78675 (15)	0.66627 (13)	0.0165 (3)
H12	0.208358	0.856744	0.588440	0.020*
C13	0.2081 (2)	0.82569 (15)	0.77770 (13)	0.0180 (3)
H13	0.192322	0.922782	0.774977	0.022*
C14	0.2212 (2)	0.72541 (15)	0.89328 (13)	0.0181 (3)
C15	0.2458 (2)	0.58249 (16)	0.89528 (13)	0.0198 (3)
H15	0.255225	0.512582	0.973156	0.024*
C16	0.2564 (2)	0.54221 (15)	0.78484 (13)	0.0178 (3)
H16	0.274169	0.444908	0.787414	0.021*
C17	0.2048 (3)	0.76846 (17)	1.01452 (14)	0.0244 (3)
H17A	0.213608	0.868262	0.993749	0.029*
H17B	0.316062	0.708018	1.058750	0.029*
C18	0.0129 (3)	0.7546 (2)	1.10285 (16)	0.0313 (4)
H18A	−0.097706	0.812084	1.058595	0.047*
H18B	0.005407	0.788052	1.178329	0.047*
H18C	0.007697	0.654765	1.128448	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0318 (6)	0.0145 (5)	0.0139 (5)	−0.0080 (4)	−0.0037 (4)	−0.0041 (4)
O2	0.0335 (6)	0.0191 (5)	0.0158 (5)	−0.0097 (4)	−0.0050 (4)	−0.0038 (4)
O3	0.0413 (6)	0.0133 (5)	0.0183 (5)	−0.0077 (4)	−0.0089 (4)	−0.0034 (4)
N1	0.0710 (12)	0.0230 (7)	0.0202 (7)	−0.0198 (7)	−0.0045 (7)	−0.0038 (5)
N2	0.0323 (7)	0.0165 (6)	0.0140 (5)	−0.0083 (5)	−0.0042 (5)	−0.0052 (4)
C1	0.0364 (8)	0.0162 (6)	0.0184 (7)	−0.0089 (6)	−0.0048 (6)	−0.0050 (5)
C3	0.0167 (6)	0.0147 (6)	0.0147 (6)	−0.0038 (4)	−0.0032 (4)	−0.0036 (5)
C4	0.0185 (6)	0.0147 (6)	0.0139 (6)	−0.0060 (5)	−0.0017 (5)	−0.0037 (5)
C5	0.0160 (6)	0.0142 (6)	0.0137 (6)	−0.0041 (4)	−0.0020 (4)	−0.0026 (5)
C6	0.0176 (6)	0.0153 (6)	0.0146 (6)	−0.0043 (5)	−0.0030 (5)	−0.0041 (5)
C7	0.0184 (6)	0.0159 (6)	0.0147 (6)	−0.0045 (5)	−0.0037 (5)	−0.0043 (5)
C8	0.0197 (6)	0.0138 (6)	0.0176 (6)	−0.0038 (5)	−0.0051 (5)	−0.0045 (5)
C9	0.0466 (10)	0.0154 (7)	0.0241 (7)	−0.0066 (6)	−0.0131 (7)	−0.0067 (6)
C10	0.0396 (10)	0.0355 (10)	0.0414 (10)	−0.0102 (8)	−0.0068 (8)	−0.0145 (8)
C11	0.0158 (6)	0.0149 (6)	0.0148 (6)	−0.0053 (4)	−0.0025 (4)	−0.0041 (5)
C12	0.0198 (6)	0.0146 (6)	0.0156 (6)	−0.0053 (5)	−0.0034 (5)	−0.0029 (5)
C13	0.0235 (6)	0.0155 (6)	0.0171 (6)	−0.0079 (5)	−0.0019 (5)	−0.0047 (5)
C14	0.0224 (6)	0.0202 (7)	0.0147 (6)	−0.0101 (5)	−0.0008 (5)	−0.0054 (5)
C15	0.0269 (7)	0.0190 (6)	0.0139 (6)	−0.0093 (5)	−0.0028 (5)	−0.0011 (5)
C16	0.0225 (6)	0.0148 (6)	0.0167 (6)	−0.0072 (5)	−0.0024 (5)	−0.0026 (5)
C17	0.0389 (8)	0.0253 (7)	0.0151 (6)	−0.0173 (6)	−0.0023 (6)	−0.0057 (5)
C18	0.0311 (8)	0.0440 (10)	0.0187 (7)	−0.0055 (7)	−0.0023 (6)	−0.0126 (7)

Geometric parameters (Å, º)

O1—C5	1.3600 (16)	C10—H10B	0.9800
O1—N2	1.3940 (15)	C10—H10C	0.9800
O2—C8	1.2033 (17)	C11—C12	1.3973 (18)
O3—C8	1.3319 (17)	C11—C16	1.4016 (18)
O3—C9	1.4573 (18)	C12—C13	1.3907 (19)
N1—C1	1.148 (2)	C12—H12	0.9500
N2—C3	1.3244 (18)	C13—C14	1.3935 (19)
C1—C7	1.434 (2)	C13—H13	0.9500
C3—C4	1.4260 (18)	C14—C15	1.402 (2)
C3—C6	1.4542 (18)	C14—C17	1.507 (2)
C4—C5	1.3594 (18)	C15—C16	1.385 (2)
C4—H4	0.9500	C15—H15	0.9500
C5—C11	1.4602 (18)	C16—H16	0.9500
C6—C7	1.3417 (19)	C17—C18	1.523 (2)
C6—H6	0.9500	C17—H17A	0.9900
C7—C8	1.5023 (19)	C17—H17B	0.9900
C9—C10	1.456 (3)	C18—H18A	0.9800
C9—H9A	0.9900	C18—H18B	0.9800
C9—H9B	0.9900	C18—H18C	0.9800
C10—H10A	0.9800		

O1···H12	2.52	C1···C4	3.069 (2)
O1···H9A^{i}	2.66	C3···C11^{iv}	3.403 (2)
O2···H9B	2.38	C6···C11^{iv}	3.385 (2)
O2···H15^{ii}	2.61	C6···C16^{iv}	3.404 (2)
O2···H6	2.48	C1···H4	2.63
N1···H13^{iii}	2.65	C4···H16	2.82
N1···H4	2.65	H13···H17A	2.37
N2···H9A^{i}	2.69		

C5—O1—N2	109.17 (10)	H10A—C10—H10C	109.5
C8—O3—C9	116.59 (12)	H10B—C10—H10C	109.5
C3—N2—O1	105.59 (11)	C12—C11—C16	119.36 (12)
N1—C1—C7	178.45 (18)	C12—C11—C5	121.30 (12)
N2—C3—C4	111.53 (12)	C16—C11—C5	119.33 (12)
N2—C3—C6	115.97 (12)	C13—C12—C11	119.68 (13)
C4—C3—C6	132.48 (13)	C13—C12—H12	120.2
C5—C4—C3	104.09 (12)	C11—C12—H12	120.2
C5—C4—H4	128.0	C12—C13—C14	121.44 (13)
C3—C4—H4	128.0	C12—C13—H13	119.3
C4—C5—O1	109.62 (12)	C14—C13—H13	119.3
C4—C5—C11	133.27 (12)	C13—C14—C15	118.46 (13)
O1—C5—C11	117.11 (11)	C13—C14—C17	121.33 (13)
C7—C6—C3	127.35 (13)	C15—C14—C17	120.20 (13)
C7—C6—H6	116.3	C16—C15—C14	120.67 (13)
C3—C6—H6	116.3	C16—C15—H15	119.7
C6—C7—C1	122.94 (13)	C14—C15—H15	119.7
C6—C7—C8	119.39 (12)	C15—C16—C11	120.38 (13)
C1—C7—C8	117.67 (12)	C15—C16—H16	119.8
O2—C8—O3	126.28 (13)	C11—C16—H16	119.8
O2—C8—C7	123.60 (12)	C14—C17—C18	112.18 (13)
O3—C8—C7	110.12 (12)	C14—C17—H17A	109.2
C10—C9—O3	110.18 (14)	C18—C17—H17A	109.2
C10—C9—H9A	109.6	C14—C17—H17B	109.2
O3—C9—H9A	109.6	C18—C17—H17B	109.2
C10—C9—H9B	109.6	H17A—C17—H17B	107.9
O3—C9—H9B	109.6	C17—C18—H18A	109.5
H9A—C9—H9B	108.1	C17—C18—H18B	109.5
C9—C10—H10A	109.5	H18A—C18—H18B	109.5
C9—C10—H10B	109.5	C17—C18—H18C	109.5
H10A—C10—H10B	109.5	H18A—C18—H18C	109.5
C9—C10—H10C	109.5	H18B—C18—H18C	109.5

C5—O1—N2—C3	−0.13 (15)	C1—C7—C8—O3	−4.46 (18)
O1—N2—C3—C4	0.20 (15)	C8—O3—C9—C10	91.16 (17)
O1—N2—C3—C6	−178.31 (11)	C4—C5—C11—C12	−166.21 (15)
N2—C3—C4—C5	−0.19 (16)	O1—C5—C11—C12	14.54 (19)
C6—C3—C4—C5	177.99 (14)	C4—C5—C11—C16	15.0 (2)

C3—C4—C5—O1	0.10 (15)	O1—C5—C11—C16	−164.26 (12)
C3—C4—C5—C11	−179.19 (14)	C16—C11—C12—C13	−0.6 (2)
N2—O1—C5—C4	0.02 (15)	C5—C11—C12—C13	−179.36 (12)
N2—O1—C5—C11	179.44 (11)	C11—C12—C13—C14	−0.1 (2)
N2—C3—C6—C7	179.15 (14)	C12—C13—C14—C15	0.4 (2)
C4—C3—C6—C7	1.0 (2)	C12—C13—C14—C17	−178.16 (13)
C3—C6—C7—C1	1.9 (2)	C13—C14—C15—C16	−0.1 (2)
C3—C6—C7—C8	−177.75 (12)	C17—C14—C15—C16	178.47 (14)
C9—O3—C8—O2	0.6 (2)	C14—C15—C16—C11	−0.5 (2)
C9—O3—C8—C7	−179.66 (12)	C12—C11—C16—C15	0.9 (2)
C6—C7—C8—O2	−5.0 (2)	C5—C11—C16—C15	179.68 (13)
C1—C7—C8—O2	175.34 (14)	C13—C14—C17—C18	109.02 (16)
C6—C7—C8—O3	175.16 (13)	C15—C14—C17—C18	−69.51 (19)

Symmetry codes: (i) x, y+1, z; (ii) x, y, z−1; (iii) x, y−1, z; (iv) −x+1, −y+1, −z+1.