2-Azido-N-(4-methylphenyl)acetamide

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The asymmetric unit of the title compound, C۹H۱۰N۴O, comprises three independent molecules, two pairs of which differ significantly in the rotational orientation of the azido group and one pair having very similar conformations; the N—N—C—C torsion angles are −173.9 (2), −102.7 (2) and −173.6 (2)°. In the crystal, each independent molecule forms N—H···O hydrogen bonds with its glide-plane-related counterparts, forming zigzag chains extending along the c-axis direction.

Structure description

N-arylacetamides are significant intermediates for the synthesis of medicinal, agrochemical and pharmaceutical compounds (Beccalli et al., 2007; Valeur & Bradley, 2009; Allen & Williams, 2011; Missioui et al., 2021, 2022a,b). Azides have found valuable applications in medicinal chemistry (Contin et al., 2019), molecular biology (Ahmed & Abdallah, 2019) and attract increasing attention in the field of organic synthesis as intermediates for the preparation of heterocycles such as tetrazoles, triazolines, triazoles, etc (Chauhan et al., 2019; Bakulev et al., 2019; Abad et al., 2020; Missioui, Lgaz et al., 2022). Based on the aforementioned information and in continuation of our research efforts to synthesize more N-arylacetamides (Missioui et al., 2020; Missioui, Guerrab, Nchioua et al., 2022; Guerrab et al., 2021), we report the synthesis and crystal structure of the title compound. The structure of the closely related compound 2-azido-N-(4-fluorophenyl)acetamide is reported by Missioui, Guerrab, Alsubari et al. (2022).

The asymmetric unit comprises three independent molecules with the azide moieties oriented in opposite directions between molecules containing O1 and O2 but with the same situation in the molecules containing O2 and O3 (Table 1). On the other hand, the...
molecules containing O1 and O3 have very similar conformations. The rotational orientations of the phenyl groups with respect to the carboxamide moieties are partially determined by intramolecular C—H...O hydrogen bonds (Fig. 1 and Table 2).

In the crystal, each component of the asymmetric unit forms a chain with its counterparts related by the glide plane and extending along the c-axis direction through N1—H1A...O1i or N5—H5A...O2i or N9—H9C...O3i hydrogen bonds (Table 2). In the case of the molecule containing O2, the chain is reinforced by C18—H18B...O2 hydrogen bonds (Table 2 and Figs. 2 and 3). The chains pack through normal van der Waals contacts.

Synthesis and crystallization

2-Chloro-N-(p-tolyl)acetamide (0.011 mol) and sodium azide (0.015 mol) were dissolved in a mixture of ethanol/water (70:30) then refluxed for 24 h at 80°C. After completion of the reaction (monitored by thin-layer chromatography, TLC), the 2-azido-N-(4-methylphenyl)acetamide precipitate was filtered and washed with cold water. A portion of the product was dissolved in hot ethanol, the solution was filtered and the filtrate was left undisturbed for 7 days to form colourless plate-like crystals. Yield 73%, mp 360–362 K, FT–IR (ATR, cm⁻¹) 3254 ν(N—H amide), 3073 ν(C—H arom), 2961 ν(C—H,CH₃), 2109 ν(N₃), 1027 ν(N—C amide), 1660 ν(C==O amide), 1175 ν(C—N). ¹H NMR (DMSO–d₆) p.p.m. 4.02 (2H, s, CH₂), 4.21 (3H, s, CH₃), 6.93–7.1 (4H, m, J = 1.3 Hz, H_arom), 10.05 (1H, s, NH). ¹³C NMR (DMSO–d₆) δ p.p.m. 51.18 (CH₂), 63.85 (CH₃), 131.47 (C_arom—N), 155.47 (C_arom—O), 113.90–120.86 (C_arom);
data reports

Table 3

Experimental details.

| Crystal data | Chemical formula | C_{9}H_{10}N_{4}O |
|--------------|------------------|------------------|
| M_r          | 190.21           |                  |
| Crystal system, space group | Monoclinic, P2_1/c |
| Temperature (K) | 150             |
| a, b, c (Å)  | 14.4362 (4), 21.3403 (6), 9.2949 (3) |
| β (°)        | 98.356 (1)       |
| V (Å³)       | 2833.11 (14)     |
| Z            | 12               |
| Radiation type | Cu Kα            |
| μ (mm⁻¹)     | 0.77             |
| Crystal size (mm) | 0.22 × 0.16 × 0.08 |

Data collection

Diffractometer | Bruker D8 VENTURE PHOTON 100 CMOS |

Absorption correction | Multi-scan (SADABS; Krause et al., 2015) |

Tmin, Tmax | 0.86, 0.94 |

No. of measured, independent and observed r>2σ(I) reflections | 21650, 5486, 4161 |

Rint | 0.039 |

(sinθ/λ)max (Å⁻¹) | 0.617 |

Refinement

R(F² > 2σ(F²)), wR(F²), S | 0.059, 0.178, 1.05 |

No. of parameters | 466 |

H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |

Δρmax, Δρmin (e Å⁻³) | 0.44, –0.39 |

Computer programs: APEX3 and SAINT (Bruker, 2016), SHELXT (Sheldrick, 2015a), SHELXL 2018/1 (Sheldrick, 2015b), DIAMOND (Brandenburg & Putz, 2012) and SHELXTL (Sheldrick, 2008).

165.71 (C=O); HRMS (ESI MS) (m/z) calculated for C_{9}H_{10}N_{4}O found 190.21 found 190.1191.

Refinement

Crystal data, data collection and structure and refinement details are summarized in Table 3.

Acknowledgements

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full crystallographic data

IUCrData (2022). 7, x220621  [https://doi.org/10.1107/S2414314622006216]

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Crystal data

C₉H₁₀N₄O
Mᵣ = 190.21
Monoclinic, P₂₁/c
a = 14.4362 (4) Å
b = 21.3403 (6) Å
c = 9.2949 (3) Å
β = 98.356 (1)°
V = 2833.11 (14) Å³
Z = 12

F(000) = 1200
Dₐ = 1.338 Mg m⁻³
Cu Kα radiation, λ = 1.54178 Å

Cell parameters from 9919 reflections
θ = 3.7–72.2°
µ = 0.77 mm⁻¹
T = 150 K
Plate, colourless

0.22 × 0.16 × 0.08 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IµS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm⁻¹
ω scans
(Absorption correction: multi-scan (SADABS; Krause et al., 2015))

21650 measured reflections
5486 independent reflections
4161 reflections with I > 2σ(I)

R(int) = 0.039
θ(max) = 72.2°, θ(min) = 3.7°
h = −17→17
k = −26→24
l = −10→11

Refinement

Refinement on F²
Least-squares matrix: full
R[F² > 2σ(F²)] = 0.059
wR(F²) = 0.178
S = 1.05
5486 reflections
466 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
w = 1/[σ²(F⁰) + (0.0988P)² + 1.2801P]
where P = (F² + 2Fc²)/3

(Δ/σ)max = 0.002
Δρ(max) = 0.44 e Å⁻³
Δρ(min) = −0.39 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 F² against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F², conventional R-factors R are based on F, with F set to zero for negative F². The threshold expression of F² > 2σ(F²) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F² are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger. The methyl group hydrogen atoms were included as riding contributions in idealized positions since independent refinement yielded unsatisfactory geometries.

The H atoms were treated by a mixture of independent and constrained refinement.

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

|       | x     | y     | z     | Uiso * / Ueq |
|-------|-------|-------|-------|--------------|
| O1    | 0.94983(12) | 0.27610(7) | 0.28617(15) | 0.0374(4) |
| N1    | 0.94218(12) | 0.29612(8)  | 0.04434(18)  | 0.0288(4)  |
| H1A   | 0.9534(17)  | 0.2808(11)  | −0.037(3)    | 0.036(6)*  |
| N2    | 1.06934(16) | 0.17717(11) | 0.2860(2)    | 0.0456(5)  |
| N3    | 1.12261(17) | 0.14178(11) | 0.2867(2)    | 0.0462(5)  |
| N4    | 1.18070(17) | 0.10247(12) | 0.3057(3)    | 0.0584(6)  |
| C1    | 0.87815(13) | 0.34695(9)  | 0.0273(2)    | 0.0271(4)  |
| C2    | 0.82911(16) | 0.35703(10) | −0.1109(2)   | 0.0342(5)  |
| H2    | 0.8403(17)  | 0.3316(11)  | −0.190(3)    | 0.036(6)*  |
| C3    | 0.76610(16) | 0.40609(11) | −0.1351(3)   | 0.0395(5)  |
| H3    | 0.7357(18)  | 0.4126(12)  | −0.230(3)    | 0.044(7)*  |
| C4    | 0.75000(15) | 0.44650(10) | −0.0236(3)   | 0.0361(5)  |
| C5    | 0.80085(16) | 0.43586(10) | 0.1134(3)    | 0.0358(5)  |
| H5    | 0.7923(17)  | 0.4632(12)  | 0.195(3)     | 0.040(7)*  |
| C6    | 0.86475(16) | 0.38713(10) | 0.1402(2)    | 0.0324(5)  |
| H6    | 0.8968(18)  | 0.3818(12)  | 0.240(3)     | 0.051(8)*  |
| C7    | 0.68108(17) | 0.49939(12) | −0.0490(3)   | 0.0491(6)  |
| H7A   | 0.684547    | 0.518373    | −0.144064    | 0.074*     |
| H7B   | 0.695979    | 0.531009    | 0.027316     | 0.074*     |
| H7C   | 0.617706    | 0.483320    | −0.046823    | 0.074*     |
| C8    | 0.97286(14) | 0.26489(9)  | 0.1665(2)    | 0.0278(4)  |
| C9    | 1.04041(16) | 0.21228(10) | 0.1437(2)    | 0.0328(5)  |
| H9A   | 1.094(2)    | 0.2312(13)  | 0.113(3)     | 0.051(8)*  |
| H9B   | 1.0123(18)  | 0.1829(13)  | 0.072(3)     | 0.046(7)*  |
| O2    | 0.59911(11) | 0.27335(7)  | 0.86318(15)  | 0.0342(4)  |
| N5    | 0.58708(12) | 0.29502(8)  | 0.62103(18)  | 0.0267(4)  |
| H5A   | 0.5974(17)  | 0.2809(11)  | 0.539(3)     | 0.036(6)*  |
| N6    | 0.68901(13) | 0.16221(9)  | 0.8282(2)    | 0.0382(4)  |
| N7    | 0.75608(14) | 0.16342(10) | 0.9230(2)    | 0.0404(5)  |
| N8    | 0.81422(19) | 0.15780(17) | 1.0172(3)    | 0.0832(10) |
| C10   | 0.52692(14) | 0.34800(9)  | 0.6098(2)    | 0.0256(4)  |
| C11   | 0.47922(14) | 0.36246(9)  | 0.4726(2)    | 0.0284(4)  |
| H11   | 0.4846(15)  | 0.3348(10)  | 0.395(3)     | 0.029(6)*  |
| C12   | 0.42233(15) | 0.41482(10) | 0.4533(2)    | 0.0333(5)  |
| H12   | 0.3878(18)  | 0.4254(12)  | 0.350(3)     | 0.044(7)*  |
| C13   | 0.41091(14) | 0.45438(9)  | 0.5689(2)    | 0.0330(5)  |
| C14   | 0.45925(16) | 0.43892(10) | 0.7051(3)    | 0.0362(5)  |
| Atom  | U_{11}   | U_{22}   | U_{33}   | U_{12}   | U_{13}   | U_{23}   |
|-------|----------|----------|----------|----------|----------|----------|
| O1    | 0.0544 (10) | 0.0360 (8) | 0.0244 (7) | 0.0067 (7) | 0.0146 (7) | 0.0036 (6) |
| N1    | 0.0348 (9) | 0.0308 (9) | 0.0221 (8) | 0.0018 (7) | 0.0092 (7) | −0.0002 (6) |
| N2    | 0.0641 (14) | 0.0517 (12) | 0.0258 (10) | 0.0102 (11) | 0.0228 (9) | 0.0092 (8) |
| N3    | 0.0592 (14) | 0.0516 (13) | 0.0277 (10) | −0.0166 (12) | 0.0066 (9) | 0.0056 (9) |
| N4    | 0.0638 (15) | 0.0573 (14) | 0.0541 (14) | 0.0200 (12) | 0.0080 (11) | 0.0149 (11) |
| C1    | 0.0274 (9) | 0.0265 (10) | 0.0287 (10) | −0.0027 (8) | 0.0083 (8) | 0.0028 (7) |
| C2    | 0.0373 (11) | 0.0365 (11) | 0.0288 (11) | −0.0003 (9) | 0.0050 (9) | −0.0025 (9) |
| C3    | 0.0377 (12) | 0.0432 (13) | 0.0359 (13) | 0.0038 (10) | −0.0009 (10) | 0.0036 (9) |
| C4    | 0.0290 (10) | 0.0327 (11) | 0.0466 (13) | −0.0024 (9) | 0.0058 (9) | 0.0012 (9) |
### Geometric parameters (Å, °)

|    | C1—C8 | 1.230 (2) | C12—H12 | 1.04 (3) |
|----|--------|-----------|----------|----------|
| N1—C8 | 1.335 (3) | C13—C14 | 1.393 (3) |
| N1—C1 | 1.419 (3) | C13—C16 | 1.501 (3) |
| N1—H1A | 0.86 (3) | C14—C15 | 1.386 (3) |
| N2—N3 | 1.077 (3) | C14—H14 | 0.95 (3) |
| N2—C9 | 1.525 (3) | C15—H15 | 0.91 (3) |
| N3—N4 | 1.181 (3) | C16—H16A | 0.9800 |
| C1—C6 | 1.390 (3) | C16—H16B | 0.9800 |
| C1—C7 | 1.390 (3) | C16—H16C | 0.9800 |
| C2—C3 | 1.384 (3) | C17—C18 | 1.528 (3) |
| C2—H2 | 0.95 (2) | C18—H18A | 1.01 (3) |
| C3—C4 | 1.394 (3) | C18—H18B | 0.99 (3) |
| Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|----------------------|--------------|----------------------|--------------|
| C3—H3                | 0.94 (3)     | O3—C26               | 1.232 (2)    |
| C4—C5                | 1.393 (3)    | N9—C26               | 1.341 (3)    |
| C4—C7                | 1.500 (3)    | N9—C19               | 1.415 (3)    |
| C5—C6                | 1.388 (3)    | N9—H9C               | 0.81 (3)     |
| C5—H5                | 0.98 (3)     | N10—N11              | 1.128 (3)    |
| C6—H6                | 0.98 (3)     | N10—C27              | 1.505 (3)    |
| C7—H7A               | 0.9800       | N11—N12              | 1.161 (3)    |
| C7—H7B               | 0.9800       | C19—C24              | 1.386 (3)    |
| C7—H7C               | 0.9800       | C19—C20              | 1.396 (3)    |
| C8—C9                | 1.522 (3)    | C20—C21              | 1.382 (3)    |
| C9—H9A               | 0.96 (3)     | C20—H20              | 0.92 (3)     |
| C9—H9B               | 0.96 (3)     | C21—C22              | 1.390 (3)    |
| O2—C17               | 1.233 (2)    | C21—H21              | 0.96 (3)     |
| N5—C17               | 1.339 (3)    | C22—C23              | 1.394 (4)    |
| N5—C10               | 1.420 (2)    | C22—C25              | 1.502 (3)    |
| N5—H5A               | 0.85 (3)     | C23—C24              | 1.384 (3)    |
| N6—N7                | 1.211 (3)    | C23—H23              | 1.03 (3)     |
| N6—C18               | 1.465 (3)    | C24—H24              | 0.91 (3)     |
| N7—N8                | 1.128 (3)    | C25—H25A             | 0.9800       |
| C10—C15              | 1.390 (3)    | C25—H25B             | 0.9800       |
| C10—C11              | 1.393 (3)    | C25—H25C             | 0.9800       |
| C11—C12              | 1.383 (3)    | C26—C27              | 1.524 (3)    |
| C11—H11              | 0.95 (2)     | C27—H27A             | 0.94 (3)     |
| C12—C13              | 1.395 (3)    | C27—H27B             | 0.93 (3)     |
| C8—N1—C1             | 127.34 (17)  | C13—C14—H14          | 115.7 (19)   |
| C8—N1—H1A            | 118.5 (16)   | C14—C15—C10          | 119.6 (2)    |
| C1—N1—H1A            | 113.2 (16)   | C14—C15—H15          | 122.6 (16)   |
| N3—N2—C9             | 117.05 (19)  | C10—C15—H15          | 117.7 (16)   |
| N2—N3—N4             | 171.7 (3)    | C13—C16—H16A         | 109.5        |
| C6—C1—C2             | 119.58 (19)  | C13—C16—H16B         | 109.5        |
| C6—C1—N1             | 123.19 (18)  | H16A—C16—H16B        | 109.5        |
| C2—C1—N1             | 117.21 (18)  | C13—C16—H16C         | 109.5        |
| C3—C2—C1             | 120.1 (2)    | H16A—C16—H16C        | 109.5        |
| C3—C2—H2             | 119.1 (15)   | H16B—C16—H16C        | 109.5        |
| C1—C2—H2             | 120.7 (15)   | O2—C17—N5            | 124.77 (18)  |
| C2—C3—C4             | 121.6 (2)    | O2—C17—C18           | 121.65 (18)  |
| C2—C3—H3             | 118.1 (16)   | N5—C17—C18           | 113.54 (16)  |
| C4—C3—H3             | 120.3 (16)   | N6—C18—C17           | 109.98 (17)  |
| C5—C4—C3             | 117.2 (2)    | N6—C18—H18A          | 110.7 (15)   |
| C5—C4—C7             | 121.0 (2)    | C17—C18—H18A         | 108.6 (15)   |
| C3—C4—C7             | 121.8 (2)    | N6—C18—H18B          | 107.3 (17)   |
| C6—C5—C4             | 122.3 (2)    | C17—C18—H18B         | 109.6 (16)   |
| C6—C5—H5             | 117.6 (15)   | H18A—C18—H18B        | 111 (2)      |
| C4—C5—H5             | 120.1 (15)   | C26—N9—C19           | 127.96 (17)  |
| C5—C6—C1             | 119.3 (2)    | C26—N9—H9C           | 114.8 (17)   |
| C5—C6—H6             | 117.8 (16)   | C19—N9—H9C           | 117.0 (17)   |
| C1—C6—H6             | 122.9 (16)   | N11—N10—C27          | 117.32 (19)  |
C4—C7—H7A 109.5  N10—N11—N12 171.3 (2)
C4—C7—H7B 109.5  C24—C19—C20 119.0 (2)
H7A—C7—H7B 109.5  C24—C19—N9 123.58 (19)
C4—C7—H7C 109.5  C20—C19—N9 117.38 (18)
H7A—C7—H7C 109.5  C21—C20—C19 120.4 (2)
C4—C7—H7C 109.5  C21—C20—H20 118.9 (17)
O1—C8—N1 124.90 (19)  C19—C20—H20 120.5 (17)
O1—C8—C9 122.14 (18)  C20—C21—C22 121.8 (2)
N1—C8—C9 112.96 (17)  C20—C21—H20 118.0 (17)
C8—C9—N2 110.01 (17)  C21—C22—C23 116.8 (2)
C8—C9—H9A 107.2 (17)  C21—C22—C25 121.7 (2)
N2—C9—H9A 109.4 (16)  C23—C22—C25 121.6 (2)
C8—C9—H9B 111.3 (16)  C23—C22—C25 121.6 (2)
O1—C8—C9 122.14 (18)  C24—C23—C22 122.5 (2)
C8—C9—N2 110.01 (17)  C24—C23—H23 124.4 (18)
C17—N5—C10 127.42 (17)  C22—C25—H25A 109.5
C17—N5—H5A 118.5 (16)  C22—C25—H25B 109.5
C10—N5—H5A 113.6 (16)  C22—C25—H25C 109.5
N7—N6—C18 115.80 (19)  C19—C24—H24 116.0 (18)
N8—N7—N6 171.4 (3)  C22—C25—H25A 109.5
C15—C10—C11 119.29 (19)  C22—C25—H25B 109.5
C15—C10—N5 123.33 (18)  C22—C25—H25C 109.5
C11—C10—N5 117.33 (17)  H25A—C25—H25C 109.5
C12—C11—C10 120.22 (19)  H25A—C25—H25B 109.5
C12—C11—H11 121.2 (14)  H25B—C25—H25C 109.5
C10—N5—C17—O2 1.3 (3)  C10—N5—C17—C18 −176.63 (18)
C10—N5—C17—C18 177.55 (19)  C10—N5—C17—O2 1.3 (3)
C1—N1—C8—O1 25.6 (3)  C13—C14—C15—C10 −0.4 (3)
C1—N1—C8—O1 25.6 (3)  C11—C10—C15—C14 0.3 (3)
N1—C1—C2—C3 1.5 (3)  N5—C10—C15—C14 177.55 (19)
C2—C3—C4—C5 −0.7 (3)  C10—N5—C17—O2 1.3 (3)
C2—C3—C4—C7 179.7 (2)  C10—N5—C17—C18 −176.63 (18)
C3—C4—C5—C6 0.1 (3)  N7—N6—C18—C17 −102.7 (2)
C3—C4—C5—C6 −179.52 (19)  C7—C4—C5—C6 179.7 (2)
C1—C2—C3—C4 0.1 (3)  C26—N9—C19—C24 14.4 (3)
C1—C2—C3—C4 −1.2 (3)  C26—N9—C19—C20 −168.4 (2)
C1—C2—C3—C4 −156.2 (2)  C24—C19—C20—C21 0.2 (3)
N1—C1—C6—C5 179.71 (19)  N9—C19—C20—C21 −177.1 (2)
C1—N1—C8—O1 −0.4 (3)  C19—C20—C21—C22 −0.2 (4)
C1—N1—C8—C9  179.19 (18)  C20—C21—C22—C23 —0.5 (4)
O1—C8—C9—N2  1.9 (3)  C20—C21—C22—C25  179.6 (2)
N1—C8—C9—N2  −177.75 (18) C21—C22—C23—C24  1.3 (3)
N3—N2—C9—C8  −173.9 (2)  C25—C22—C23—C24 −178.9 (2)
C17—N5—C10—C15  22.5 (3)  C22—C23—C24—C19 −1.3 (4)
C17—N5—C10—C11  −160.22 (19) C20—C19—C24—C23  0.5 (3)
C15—C10—C11—C12  −0.1 (3)  N9—C19—C24—C23  177.64 (19)
N5—C10—C11—C12  −177.53 (18) C19—N9—C26—O3  3.1 (3)
C10—C11—C12—C13  0.0 (3)  C19—N9—C26—C27 −176.86 (18)
C11—C12—C13—C14  −0.1 (3)  N11—N10—C27—C26 −173.6 (2)
C11—C12—C13—C16  178.9 (2)  O3—C26—C27—N10  0.8 (3)
C12—C13—C14—C15  0.2 (3)  N9—C26—C27—N10 −179.23 (18)
C16—C13—C14—C15  −178.8 (2)

### Hydrogen-bond geometry (Å, °)

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\begin{array}{cccc}
D—H···A & D—H & H···A & D···A & D—H···A \\
N1—H1A···O1i & 0.86 (3) & 2.04 (3) & 2.867 (2) & 162 (2) \\
N5—H5A···O2i & 0.85 (3) & 2.01 (3) & 2.833 (2) & 163 (2) \\
C15—H15···O2 & 0.91 (3) & 2.34 (2) & 2.905 (3) & 120 (2) \\
C18—H18B···O2j & 0.99 (3) & 2.57 (3) & 3.353 (3) & 136 (2) \\
N9—H9C···O3 & 0.81 (3) & 2.05 (3) & 2.835 (2) & 163 (2) \\
C24—H24···O3 & 0.91 (3) & 2.27 (3) & 2.882 (3) & 125 (2) \\
\end{array}
\]

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