\[ N'-(2,4-Dinitrophenyl)acetohydrazide \]

This item was submitted to Loughborough University’s Institutional Repository by the/an author.

**Citation:** ZIA-UR-REHMAN, M. ... et al, 2008. \( N'-(2,4\text{-Dinitrophenyl})\text{acetohydrazide} \). Acta Crystallographica Section E : Structure Reports Online, E64, o1441 [doi:10.1107/S1600536808019685]

**Additional Information:**

- This article was published in the journal, Acta Crystallographica Section E: Structure Reports Online [© International Union of Crystallography]. It is also available at: http://journals.iucr.org/e/

**Metadata Record:** [https://dspace.lboro.ac.uk/2134/3540](https://dspace.lboro.ac.uk/2134/3540)

**Publisher:** © International Union of Crystallography

Please cite the published version.
This item was submitted to Loughborough’s Institutional Repository by the author and is made available under the following Creative Commons Licence conditions.

For the full text of this licence, please go to:
http://creativecommons.org/licenses/by-nc-nd/2.5/
$N'$-(2,4-Dinitrophenyl)acetohydrazide

Muhammad Zia-ur-Rehman, Mark R. J. Elsegood, Shahid Mahmud and Hamid Latif Siddiqui

Acta Cryst. (2008). E64, o1441

This article is distributed under the terms of the Creative Commons Attribution Licence http://creativecommons.org/licenses/by/2.0/uk/legalcode, which permits unrestricted use, distribution, and reproduction in any medium, provided the original authors and source are cited.
In the title compound, C₈H₈N₄O₅, the nitro groups ortho and para to the hydrazone group are twisted by 10.0 (2) and 25.5 (2)°, respectively, relative to the aromatic ring. The structure exhibits an intramolecular N—H—O hydrogen bond, giving rise to chains, and weaker ONO···ONO [2.944 (2) Å] and C—H···O—N interactions linking the molecules into a three-dimensional network.

Related literature
For related literature, see: Domiano et al. (1984); Guo (2007); Li et al. (1988); Rudnicka & Osmialowska (1979); Sakamoto et al. (1993); Siddiqui et al. (2007); Zia-ur-Rehman et al. (2005, 2006).

Experimental
Crystal data

\[ V = 999.76(13) \, \text{Å}^3 \]
\[ Z = 4 \]
\[ \text{Mo } K\alpha \text{ radiation} \quad 0.57 \times 0.99 \times 0.06 \, \text{mm} \]

Data collection

<table>
<thead>
<tr>
<th>Bruker APEX2 CCD</th>
<th>11843 measured reflections</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffractometer</td>
<td>1794 independent reflections</td>
</tr>
<tr>
<td>Absorption correction: multi-scan</td>
<td></td>
</tr>
<tr>
<td>( T_{\text{min}} = 0.927, T_{\text{max}} = 0.992 )</td>
<td></td>
</tr>
</tbody>
</table>

Refinement

<table>
<thead>
<tr>
<th>( R(F^2) &gt; 2\sigma(F^2) ) = 0.030</th>
<th>( wR(F^2) = 0.078 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S = 1.03 )</td>
<td>( 1794 ) reflections</td>
</tr>
<tr>
<td>( 161 ) parameters</td>
<td></td>
</tr>
</tbody>
</table>

Hydrogen-bond geometry (Å, °)

\[ D—H···A \quad D—H···A \quad D···A \quad D—H···A \]

N3—H3···O2 0.83 (2) 2.01 (2) 2.59 (2) 127 (2)
N4—H4···O2 0.85 (2) 1.95 (2) 2.78 (1) 163 (2)
C5—H5···O4ii 1.07 (2) 1.82 (3) 2.82 (2) 155 (2)
C6—H6···O4iii 0.98 (2) 1.82 (3) 2.78 (2) 154 (2)
C7—H7···O4iii 1.00 (2) 1.83 (3) 2.79 (2) 161 (2)

Programs used: \( SADABS \) (Sheldrick, 2007); \( SHELXTL \) (Bruker, 2006); \( SAINT \) (Bruker, 2006); \( X-SEED \) (Bruker, 2006); \( PLATON \) (Spek, 2009). Structure factors have been deposited with Cambridge Crystallographic Data Centre (CCDC) as supplementary publication no. 655585.

The authors are greatful to the Pakistan Council of Scientific & Industrial Research Laboratories Complex, Lahore, for providing the necessary facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2733).

References

supplementary materials

N’-(2,4-Dinitrophenyl)acetohydrazide

M. Zia-ur-Rehman, M. R. J. Elsegood, S. Mahmud and H. L. Siddiqui

Comment

The chemistry of hydrazones has been intensely investigated in recent years due to their excellent coordinating capability (Domiano et al., 1984) and pharmacological activities (Li et al., 1988). These compounds are also being used as precursors for the efficient synthesis of various condensed heterocycles in organic chemistry (Rudnicka & Osmialowska, 1979) and as highly selective metal scavengers (Sakamoto et al., 1993) in analytical chemistry. In continuation of our ongoing work on the synthesis of various heterocyclic compounds (Zia-ur-Rehman et al., 2005, 2006; Siddiqui et al., 2007), the title compound, (I), was synthesized by reacting 2,4-dinitrophenylhydrazine with acetic anhydride.

Most of the bond lengths and angles in (I) are similar to those in related molecules (Guo, 2007). The nitro groups ortho and para to the hydrazone group are twisted out of this plane by 10.0 (2) and 3.6 (2)o, respectively. The larger twist of the ortho-nitro group arises due to the desire to form an intramolecular hydrogen bond which results in a six-membered ring (Fig. 1 and Table 1). Each molecule also forms an intermolecular N––H—O=C hydrogen bond giving rise to stacks of molecules parallel to a (Fig. 2). The hydrogen-bonded chains of (I) are further linked together into a three-dimensional network (Fig. 3) via weaker C—H⋯O—N interactions involving the nitro groups and methyl and aryl H atoms (range 2.4–2.6Å) along with some weak ONO⋯NO2 interactions [O1⋯N1i = 2.944 (2)Å; symmetry code: (i) -0.5+x, 1.5-y, 2-z].

Experimental

A mixture of 2,4-dinitrophenylhydrazine (1.981 g; 10.0 mmoles) and acetic anhydride (5.0 ml) was stirred for a period of six hours at room temperature. Then, this mixture was poured into ice cooled water and neutralized with 10% sodium bicarbonate solution. The precipitated solids were collected by filtration, washed and dried. Crystals suitable for X-ray crystallography were grown by slow evaporation of solution of the title compound in a mixture of ethanol and water (90:10); m.p. 471 K; yield: 82%.

Refinement

1255 Friedel pairs were merged. H atoms bound to C were placed in geometric positions (C—H distance = 0.95 Å for aryl-H; 0.98 Å for methyl-H) using a riding model. H atoms on N had coordinates freely refined. Uiso values were set to 1.2Ueq of the carrier atom (1.5Ueq for methyl-H).
Figures

Fig. 1. The asymmetric unit of the title compound showing the intramolecular hydrogen bond. Displacement ellipsoids are drawn at the 50% probability level.

Fig. 2. Perspective view of molecules linked via intermolecular N—H···O=C hydrogen bonds parallel to a.

Fig. 3. Perspective view of the three-dimensional crystal packing showing hydrogen-bonds and other intermolecular interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity.

N'(2,4-Dinitrophenyl)acetohydrazide

Crystal data

\[ \text{C}_8\text{H}_8\text{N}_4\text{O}_5 \quad M_r = 240.18 \]

Orthorhombic, \( P2_12_12_1 \)

Hall symbol: P 2ac 2ab

\( a = 4.8585 \) Å

\( b = 10.7703 \) Å

\( c = 19.1059 \) Å

\( V = 999.76 \) Å³

\( Z = 4 \)

\( F_{000} = 496 \)

\( D_x = 1.596 \text{ Mg m}^{-3} \)

Mo \( K\alpha \) radiation

\( \lambda = 0.71073 \) Å

Cell parameters from 3491 reflections

\( \theta = 2.9^\circ - 27.8^\circ \)

\( \mu = 0.14 \text{ mm}^{-1} \)

\( T = 150 \) (2) K

Lath, orange

\( 0.57 \times 0.09 \times 0.06 \) mm

Data collection

Bruker APEXII CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

\( T = 150(2) \) K

1794 independent reflections

1616 reflections with \( I > 2\sigma(I) \)

\( R_{\text{int}} = 0.031 \)

\( \theta_{\text{max}} = 30.6^\circ \)
\( \omega \) rotation with narrow frames scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2007)
\( T_{\text{min}} = 0.927, T_{\text{max}} = 0.992 \)
11843 measured reflections
\( \theta_{\text{min}} = 2.1^\circ \)
\( h = -6 \rightarrow 6 \)
\( k = -15 \rightarrow 15 \)
\( l = -27 \rightarrow 27 \)

Refinement

Refinement on \( F^2 \)
Secondary atom site location: all non-H atoms found by direct methods

Least-squares matrix: full
Hydrogen site location: geom except NH coords freely refined

\( R[F^2 > 2\sigma(F^2)] = 0.030 \)
H atoms treated by a mixture of independent and constrained refinement

\( wR(F^2) = 0.078 \)
where \( P = (F_{o}^2 + 2F_{c}^2)/3 \)

\( S = 1.03 \)
\( \Delta \rho_{\text{max}} = 0.27 \text{ e Å}^{-3} \)
\( \Delta \rho_{\text{min}} = -0.17 \text{ e Å}^{-3} \)

Primary atom site location: structure-invariant direct methods
Extinction correction: none

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(g) 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. 1255 Friedel pairs. Friedels merged.

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

<table>
<thead>
<tr>
<th></th>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
<th>( U_{\text{iso}}^{*}/U_{\text{eq}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>0.3396 (3)</td>
<td>0.64099 (13)</td>
<td>0.89834 (7)</td>
<td>0.0206 (3)</td>
</tr>
<tr>
<td>N1</td>
<td>0.1186 (2)</td>
<td>0.67553 (11)</td>
<td>0.94555 (6)</td>
<td>0.0239 (2)</td>
</tr>
<tr>
<td>O1</td>
<td>0.0352 (2)</td>
<td>0.78314 (10)</td>
<td>0.94499 (6)</td>
<td>0.0298 (2)</td>
</tr>
<tr>
<td>O2</td>
<td>0.0219 (2)</td>
<td>0.59512 (11)</td>
<td>0.98457 (6)</td>
<td>0.0349 (3)</td>
</tr>
<tr>
<td>C2</td>
<td>0.4679 (3)</td>
<td>0.73783 (13)</td>
<td>0.86286 (7)</td>
<td>0.0234 (3)</td>
</tr>
<tr>
<td>H2</td>
<td>0.4153</td>
<td>0.8215</td>
<td>0.8710</td>
<td>0.028*</td>
</tr>
<tr>
<td>C3</td>
<td>0.6722 (3)</td>
<td>0.70968 (14)</td>
<td>0.81593 (7)</td>
<td>0.0245 (3)</td>
</tr>
<tr>
<td>N2</td>
<td>0.8161 (3)</td>
<td>0.81093 (13)</td>
<td>0.78132 (7)</td>
<td>0.0323 (3)</td>
</tr>
<tr>
<td>O3</td>
<td>0.7483 (3)</td>
<td>0.91873 (12)</td>
<td>0.79517 (7)</td>
<td>0.0428 (3)</td>
</tr>
<tr>
<td>O4</td>
<td>1.0012 (3)</td>
<td>0.78354 (13)</td>
<td>0.73998 (7)</td>
<td>0.0462 (3)</td>
</tr>
<tr>
<td>C4</td>
<td>0.7508 (3)</td>
<td>0.58725 (15)</td>
<td>0.80240 (7)</td>
<td>0.0253 (3)</td>
</tr>
<tr>
<td>H4A</td>
<td>0.8903</td>
<td>0.5700</td>
<td>0.7689</td>
<td>0.030*</td>
</tr>
</tbody>
</table>
supplementary materials

C5  0.6255 (3)  0.49242 (13)  0.83774 (7)  0.0231 (3)
H5  0.6791  0.4093  0.8283  0.028*
C6  0.4174 (3)  0.51517 (13)  0.88817 (7)  0.0200 (3)
N3  0.3089 (3)  0.42103 (11)  0.92557 (7)  0.0243 (3)
H3  0.172 (4)  0.4329 (16)  0.9508 (10)  0.029*
N4  0.3548 (3)  0.29805 (11)  0.90659 (7)  0.0222 (2)
H4  0.518 (4)  0.2710 (16)  0.9126 (10)  0.027*
C7  0.1401 (3)  0.21961 (13)  0.91490 (7)  0.0222 (3)
O5  −0.0894 (2)  0.25786 (10)  0.93114 (6)  0.0291 (2)
C8  0.2055 (4)  0.08501 (14)  0.90370 (9)  0.0310 (3)
H8A  0.1747  0.0392  0.9473  0.047*
H8B  0.3984  0.0764  0.8895  0.047*
H8C  0.0861  0.0515  0.8669  0.047*

Atomic displacement parameters (Å²)

<table>
<thead>
<tr>
<th></th>
<th>U₁₁</th>
<th>U₂₂</th>
<th>U₃₃</th>
<th>U₁₂</th>
<th>U₁₃</th>
<th>U₂₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>0.0161 (6)</td>
<td>0.0247 (6)</td>
<td>0.0211 (6)</td>
<td>−0.0007 (5)</td>
<td>−0.0003 (5)</td>
<td>−0.0036 (5)</td>
</tr>
<tr>
<td>N1</td>
<td>0.0187 (5)</td>
<td>0.0254 (5)</td>
<td>0.0276 (6)</td>
<td>−0.0018 (5)</td>
<td>0.0007 (5)</td>
<td>−0.0083 (5)</td>
</tr>
<tr>
<td>O1</td>
<td>0.0243 (5)</td>
<td>0.0272 (5)</td>
<td>0.0380 (6)</td>
<td>0.0046 (4)</td>
<td>−0.0021 (5)</td>
<td>−0.0092 (4)</td>
</tr>
<tr>
<td>O2</td>
<td>0.0334 (6)</td>
<td>0.0304 (6)</td>
<td>0.0408 (6)</td>
<td>−0.0044 (5)</td>
<td>0.0178 (5)</td>
<td>−0.0053 (5)</td>
</tr>
<tr>
<td>C2</td>
<td>0.0218 (6)</td>
<td>0.0241 (6)</td>
<td>0.0242 (6)</td>
<td>−0.0029 (5)</td>
<td>−0.0050 (5)</td>
<td>0.0001 (5)</td>
</tr>
<tr>
<td>C3</td>
<td>0.0229 (6)</td>
<td>0.0303 (7)</td>
<td>0.0203 (6)</td>
<td>−0.0070 (6)</td>
<td>−0.0027 (5)</td>
<td>0.0046 (5)</td>
</tr>
<tr>
<td>N2</td>
<td>0.0323 (7)</td>
<td>0.0384 (7)</td>
<td>0.0262 (6)</td>
<td>−0.0125 (6)</td>
<td>−0.0069 (6)</td>
<td>0.0095 (5)</td>
</tr>
<tr>
<td>O3</td>
<td>0.0475 (8)</td>
<td>0.0320 (6)</td>
<td>0.0489 (7)</td>
<td>−0.0124 (6)</td>
<td>−0.0052 (6)</td>
<td>0.0114 (5)</td>
</tr>
<tr>
<td>O4</td>
<td>0.0430 (7)</td>
<td>0.0581 (8)</td>
<td>0.0374 (6)</td>
<td>−0.0177 (7)</td>
<td>0.0111 (6)</td>
<td>0.0105 (6)</td>
</tr>
<tr>
<td>C4</td>
<td>0.0203 (7)</td>
<td>0.0352 (7)</td>
<td>0.0203 (6)</td>
<td>−0.0025 (6)</td>
<td>0.0020 (5)</td>
<td>0.0001 (6)</td>
</tr>
<tr>
<td>C5</td>
<td>0.0205 (6)</td>
<td>0.0267 (6)</td>
<td>0.0221 (6)</td>
<td>0.0012 (5)</td>
<td>0.0029 (5)</td>
<td>−0.0024 (5)</td>
</tr>
<tr>
<td>C6</td>
<td>0.0161 (6)</td>
<td>0.0238 (6)</td>
<td>0.0200 (6)</td>
<td>−0.0007 (5)</td>
<td>−0.0006 (5)</td>
<td>−0.0014 (5)</td>
</tr>
<tr>
<td>N3</td>
<td>0.0210 (6)</td>
<td>0.0217 (5)</td>
<td>0.0301 (6)</td>
<td>0.0006 (5)</td>
<td>0.0084 (5)</td>
<td>−0.0019 (5)</td>
</tr>
<tr>
<td>N4</td>
<td>0.0154 (5)</td>
<td>0.0200 (5)</td>
<td>0.0312 (6)</td>
<td>0.0011 (4)</td>
<td>0.0006 (5)</td>
<td>−0.0004 (5)</td>
</tr>
<tr>
<td>C7</td>
<td>0.0182 (6)</td>
<td>0.0256 (6)</td>
<td>0.0228 (6)</td>
<td>−0.0011 (5)</td>
<td>−0.0022 (5)</td>
<td>0.0029 (5)</td>
</tr>
<tr>
<td>O5</td>
<td>0.0159 (5)</td>
<td>0.0339 (6)</td>
<td>0.0375 (6)</td>
<td>−0.0002 (4)</td>
<td>0.0012 (4)</td>
<td>0.0046 (5)</td>
</tr>
<tr>
<td>C8</td>
<td>0.0308 (8)</td>
<td>0.0235 (6)</td>
<td>0.0389 (8)</td>
<td>−0.0011 (6)</td>
<td>−0.0008 (7)</td>
<td>0.0019 (6)</td>
</tr>
</tbody>
</table>

Geometric parameters (Å, °)

|   |    |    | C5—C6 |    | C5—H5 |    | C6—N3 |    | C2—O4 |    | C5—H8A |    | C7—O5 |    | C7—C8 |    | N2—O4 |    | C8—C8 |    | C4—C5 |    |
|---|---|---|-------|---|-------|---|-------|---|-------|---|-------|---|-------|---|-------|---|-------|---|-------|---|
| C1—C2 | 1.3915 (19) | C5—C6 | 1.4178 (18) |
| C1—C6 | 1.4202 (19) | C5—H5 | 0.9500 |
| C1—N1 | 1.4508 (18) | C6—N3 | 1.3477 (18) |
| N1—O1 | 1.2278 (16) | N3—N4 | 1.3913 (17) |
| N1—O2 | 1.2354 (16) | N3—H3 | 0.83 (2) |
| C2—C3 | 1.371 (2) | N4—C7 | 1.3519 (18) |
| C2—H2 | 0.9500 | N4—H4 | 0.85 (2) |
| C3—C4 | 1.397 (2) | C7—O5 | 1.2282 (17) |
| C3—N2 | 1.4543 (19) | C7—C8 | 1.500 (2) |
| N2—O4 | 1.233 (2) | C8—H8A | 0.9800 |
| N2—O3 | 1.2355 (19) | C8—H8B | 0.9800 |
| C4—C5 | 1.367 (2) | C8—H8C | 0.9800 |

sup-4
**supplementary materials**

<table>
<thead>
<tr>
<th>Bond</th>
<th>Distance (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C4—H4A</td>
<td>0.9500</td>
</tr>
<tr>
<td>C2—C1—C6</td>
<td>121.96 (13)</td>
</tr>
<tr>
<td>C2—C1—N1</td>
<td>116.25 (12)</td>
</tr>
<tr>
<td>C6—C1—N1</td>
<td>121.79 (12)</td>
</tr>
<tr>
<td>O1—N1—O2</td>
<td>122.79 (12)</td>
</tr>
<tr>
<td>O1—N1—C1</td>
<td>118.74 (12)</td>
</tr>
<tr>
<td>O2—N1—C1</td>
<td>118.47 (12)</td>
</tr>
<tr>
<td>C3—C2—C1</td>
<td>118.50 (13)</td>
</tr>
<tr>
<td>C3—C2—H2</td>
<td>120.8</td>
</tr>
<tr>
<td>C1—C2—H2</td>
<td>120.8</td>
</tr>
<tr>
<td>C2—C3—C4</td>
<td>121.83 (13)</td>
</tr>
<tr>
<td>C2—C3—N2</td>
<td>118.65 (14)</td>
</tr>
<tr>
<td>C4—C3—N2</td>
<td>119.49 (13)</td>
</tr>
<tr>
<td>O4—N2—O3</td>
<td>123.81 (14)</td>
</tr>
<tr>
<td>O4—N2—C3</td>
<td>117.56 (14)</td>
</tr>
<tr>
<td>O3—N2—C3</td>
<td>118.63 (15)</td>
</tr>
<tr>
<td>C5—C4—C3</td>
<td>119.47 (13)</td>
</tr>
<tr>
<td>C5—C4—H4A</td>
<td>120.3</td>
</tr>
<tr>
<td>C3—C4—H4A</td>
<td>120.3</td>
</tr>
<tr>
<td>C4—C5—C6</td>
<td>121.60 (13)</td>
</tr>
<tr>
<td>C4—C5—H5</td>
<td>119.2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Bond</th>
<th>Distance (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C2—C1—N1—O1</td>
<td>9.02 (18)</td>
</tr>
<tr>
<td>C6—C1—N1—O1</td>
<td>−170.04 (13)</td>
</tr>
<tr>
<td>C2—C1—N1—O2</td>
<td>−171.10 (12)</td>
</tr>
<tr>
<td>C6—C1—N1—O2</td>
<td>9.84 (19)</td>
</tr>
<tr>
<td>C6—C1—C2—C3</td>
<td>1.1 (2)</td>
</tr>
<tr>
<td>N1—C1—C2—C3</td>
<td>−177.94 (12)</td>
</tr>
<tr>
<td>C1—C2—C3—C4</td>
<td>0.9 (2)</td>
</tr>
<tr>
<td>C1—C2—C3—N2</td>
<td>−177.00 (13)</td>
</tr>
<tr>
<td>C2—C3—N2—O4</td>
<td>179.13 (13)</td>
</tr>
<tr>
<td>C4—C3—N2—O4</td>
<td>1.2 (2)</td>
</tr>
<tr>
<td>C2—C3—N2—O3</td>
<td>−0.3 (2)</td>
</tr>
<tr>
<td>C4—C3—N2—O3</td>
<td>−178.27 (14)</td>
</tr>
<tr>
<td>C2—C3—C4—C5</td>
<td>−1.3 (2)</td>
</tr>
</tbody>
</table>

**Hydrogen-bond geometry (Å, °)**

<table>
<thead>
<tr>
<th>Bond</th>
<th>D—H—A</th>
<th>H···A</th>
<th>D···A</th>
<th>D—H···A</th>
</tr>
</thead>
<tbody>
<tr>
<td>N3—H3···O2</td>
<td>0.83 (2)</td>
<td>2.001 (18)</td>
<td>2.5942 (16)</td>
<td>127.9 (16)</td>
</tr>
<tr>
<td>N4—H4···O5i</td>
<td>0.85 (2)</td>
<td>1.95 (2)</td>
<td>2.7748 (16)</td>
<td>164.0 (17)</td>
</tr>
<tr>
<td>C5—H5···O4ii</td>
<td>0.95</td>
<td>2.44</td>
<td>3.249 (2)</td>
<td>143</td>
</tr>
<tr>
<td>C8—H8A···O2iii</td>
<td>0.98</td>
<td>2.58</td>
<td>3.269 (2)</td>
<td>128</td>
</tr>
<tr>
<td>C8—H8C···O3iv</td>
<td>0.98</td>
<td>2.57</td>
<td>3.527 (2)</td>
<td>165</td>
</tr>
</tbody>
</table>

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

Fig. 1
Fig. 2
supplementary materials

Fig. 3