



Crystal structures of the two isomeric hydrogen-bonded cocrystals 2-chloro-4-nitrobenzoic acid–5-nitroquinoline (1/1) and 5-chloro-2-nitrobenzoic acid–5-nitroquinoline (1/1)

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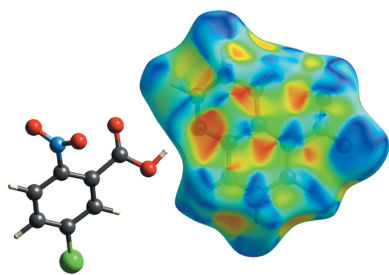
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The structures of two isomeric compounds of 5-nitroquinoline with chloro- and nitro-substituted benzoic acid, namely, 2-chloro-4-nitrobenzoic acid–5-nitroquinoline (1/1), (I), and 5-chloro-2-nitrobenzoic acid–5-nitroquinoline (1/1), (II), both $C_7H_4ClNO_4 \cdot C_9H_6N_2O_2$, have been determined at 190 K. In each compound, the acid and base molecules are held together by an $O-H \cdots N$ hydrogen bond. In the crystal of (I), the hydrogen-bonded acid–base units are linked by a $C-H \cdots O$ hydrogen bond, forming a tape structure along $[1\bar{2}0]$. The tapes are stacked into a layer parallel to the ab plane *via* $N-O \cdots \pi$ interactions between the nitro group of the base molecule and the quinoline ring system. The layers are further linked by other $C-H \cdots O$ hydrogen bonds, forming a three-dimensional network. In the crystal of (II), the hydrogen-bonded acid–base units are linked into a wide ribbon structure running along $[1\bar{1}0]$ *via* $C-H \cdots O$ hydrogen bonds. The ribbons are further linked *via* another $C-H \cdots O$ hydrogen bond, forming a layer parallel to (110). Weak $\pi-\pi$ interactions [centroid–centroid distances of 3.7080 (10) and 3.7543 (9) Å] are observed between the quinoline ring systems of adjacent layers. Hirshfeld surfaces for the 5-nitroquinoline molecules of the two compounds mapped over shape index and d_{norm} were generated to visualize the weak intermolecular interactions.

1. Chemical context

The properties of hydrogen bonds formed between organic acids and organic bases depend on the pK_a values of the acids and bases, as well as the intermolecular interactions in the crystals. For the system of quinoline and chloro- and nitro-substituted benzoic acids, we have shown that three compounds of quinoline with 3-chloro-2-nitrobenzoic acid, 4-chloro-2-nitrobenzoic acid and 5-chloro-2-nitrobenzoic acid, the ΔpK_a [$pK_a(\text{base}) - pK_a(\text{acid})$] values of which are 3.08, 2.93 and 3.04, respectively, have a short double-well $O \cdots H \cdots N$ hydrogen bond between the carboxy O atom and the aromatic N atom (Gotoh & Ishida, 2009). Similar $O \cdots H \cdots N$ hydrogen bonds have also been observed in compounds of phthalazine with 3-chloro-2-nitrobenzoic acid and 4-chloro-2-nitrobenzoic acid with ΔpK_a values of 1.65 and 1.50, respectively (Gotoh & Ishida, 2011*a*), and of isoquinoline with 3-chloro-2-nitrobenzoic acid with $\Delta pK_a = 3.58$ (Gotoh & Ishida, 2015). On the other hand, in 2-chloro-4-nitrobenzoic acid–quinoline (1/1) with $\Delta pK_a = 2.86$ (Gotoh & Ishida, 2011*b*), 3-chloro-2-nitrobenzoic acid–5-nitroquinoline (1/1) with $\Delta pK_a = 0.98$, 3-chloro-2-nitrobenzoic acid–6-nitroquinoline (1/1) with $\Delta pK_a = 1.42$ and 8-hydroxyquinolinium 3-chloro-2-nitrobenzoate with $\Delta pK_a = 3.02$ (Gotoh & Ishida,



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

$Cg3$ and $Cg4$ are the centroids of the C11–C16 ring and the N2/C8–C16 ring system, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1 \cdots N2	1.02 (8)	1.58 (7)	2.585 (5)	168 (7)
C8–H8 \cdots O2 ⁱ	0.95	2.59	3.174 (6)	120
C9–H9 \cdots O2 ⁱ	0.95	2.56	3.152 (6)	120
C13–H13 \cdots O4 ⁱⁱ	0.95	2.52	3.289 (6)	138
N3–O5 \cdots $Cg3$ ⁱⁱⁱ	1.23 (1)	3.06 (1)	3.724 (4)	113 (1)
N3–O5 \cdots $Cg4$ ⁱⁱⁱ	1.23 (1)	3.25 (1)	4.118 (4)	128 (1)

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

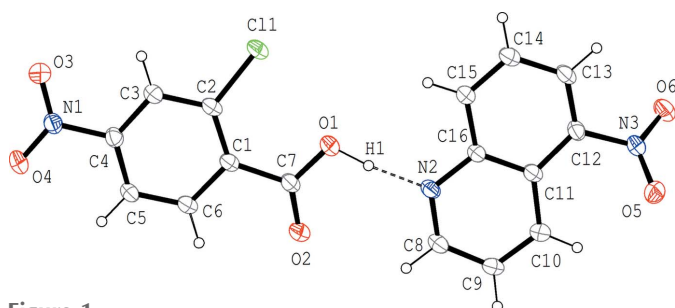


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. The O–H \cdots N hydrogen bond is indicated by a dashed line.

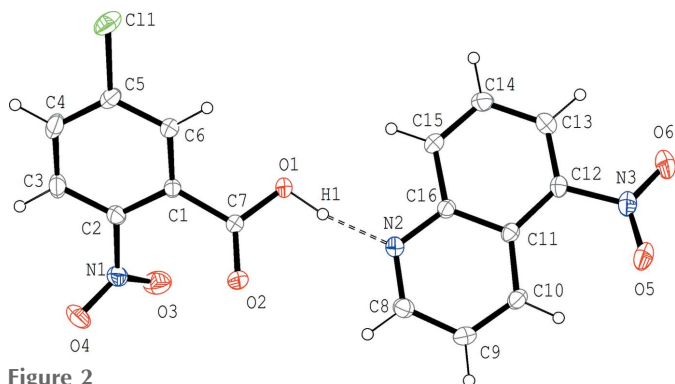


Figure 2
The molecular structure of (II), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. The O–H \cdots N hydrogen bond is indicated by a dashed line.

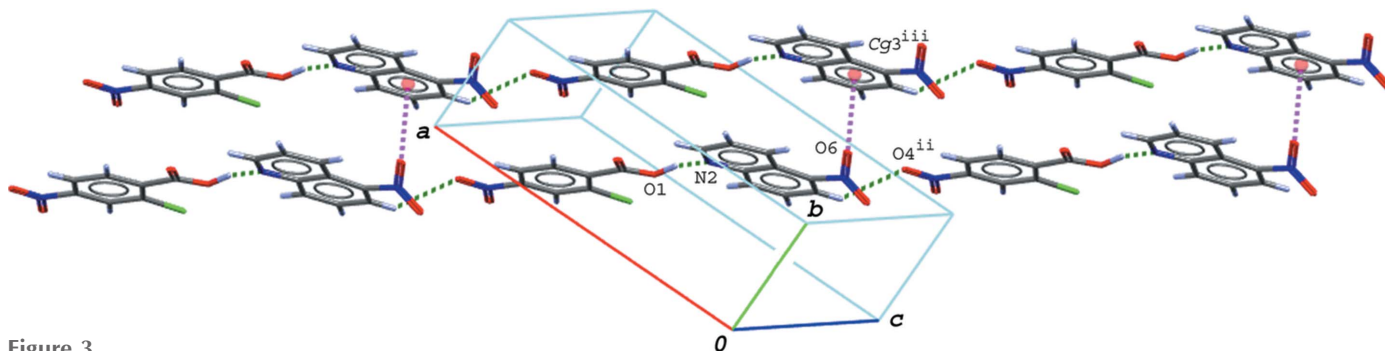


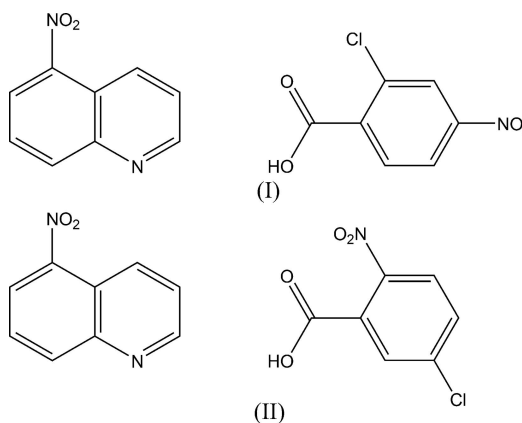
Figure 3
A packing diagram of (I), showing the hydrogen-bonded tape structure formed *via* O–H \cdots N and C–H \cdots O hydrogen bonds (green dashed lines), and N–O \cdots π interactions (magenta dashed lines) between the tapes. The N–O \cdots π interactions including the centroid of the ten-membered quinoline ring system ($Cg4$) have been omitted for clarity. [Symmetry codes: (ii) $x - 1, y + 2, z$; (iii) $x, y + 1, -z + 1$.]

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1 \cdots N2	0.99 (4)	1.66 (4)	2.6405 (17)	169 (3)
C3–H3 \cdots O4 ⁱ	0.95	2.49	3.408 (3)	162
C10–H10 \cdots O3 ⁱⁱ	0.95	2.54	3.254 (2)	132
C13–H13 \cdots O2 ⁱⁱⁱ	0.95	2.59	3.190 (2)	121
C14–H14 \cdots O2 ⁱⁱⁱ	0.95	2.56	3.173 (2)	122

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

2019), such a short disordered hydrogen bond was not observed, suggesting that the strength of the hydrogen bond between the acid O atom and the base N atom is strongly influenced by other weak intermolecular interactions.



We report here the crystal structures of the isomeric compounds 2-chloro-4-nitrobenzoic acid–5-nitroquinoline (1/1) ($\Delta pK_a = 0.76$) and 5-chloro-2-nitrobenzoic acid–5-nitroquinoline (1/1) ($\Delta pK_a = 0.94$), in order to extend our studies of short hydrogen bonding and weak intermolecular interactions in the quinoline derivative–chloro- and nitro-substituted benzoic acid system.

2. Structural commentary

Compound (I) crystallizes in the noncentrosymmetric space group $P2_1$, where the acid and base molecules are held to-

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_7H_4ClNO_4 \cdot C_9H_6N_2O_2$	$C_7H_4ClNO_4 \cdot C_9H_6N_2O_2$
M_r	375.72	375.72
Crystal system, space group	Monoclinic, $P2_1$	Triclinic, $P\bar{1}$
Temperature (K)	190	190
a, b, c (Å)	12.8265 (13), 4.7699 (5), 13.5033 (16)	7.6682 (6), 8.6515 (8), 12.8609 (10)
α, β, γ (°)	90, 109.713 (3), 90	79.170 (3), 78.968 (2), 70.394 (3)
V (Å ³)	777.73 (15)	781.80 (11)
Z	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm ⁻¹)	0.29	0.29
Crystal size (mm)	0.37 × 0.18 × 0.10	0.26 × 0.20 × 0.18
Data collection		
Diffractometer	Rigaku R-Axis RAPID	Rigaku R-Axis RAPID
Absorption correction	Numerical (NUMABS; Higashi, 1999)	Numerical (NUMABS; Higashi, 1999)
T_{min}, T_{max}	0.913, 0.972	0.933, 0.950
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14435, 4168, 2859	9772, 4502, 3075
R_{int}	0.058	0.055
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.703	0.703
Refinement		
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.056, 0.169, 1.05	0.052, 0.148, 1.09
No. of reflections	4168	4502
No. of parameters	239	239
No. of restraints	1	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.34, -0.65	0.42, -0.39
Absolute structure	Flack x determined using 898 quotients [$(I^-) - (I^+)$]/[$(I^-) + (I^+)$] (Parsons <i>et al.</i> , 2013)	-
Absolute structure parameter	0.01 (6)	-

Computer programs: *PROCESS-AUTO* (Rigaku, 2006), *SHELXT2018* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), *CrystalStructure* (Rigaku, 2018) and *PLATON* (Spek, 2015).

ther by an O—H···N hydrogen bond between the carboxy group and the N atom of the base (Fig. 1 and Table 1). The

hydrogen-bonded acid–base unit is approximately planar; the quinoline ring system (N2/C8–C16) makes dihedral angles of

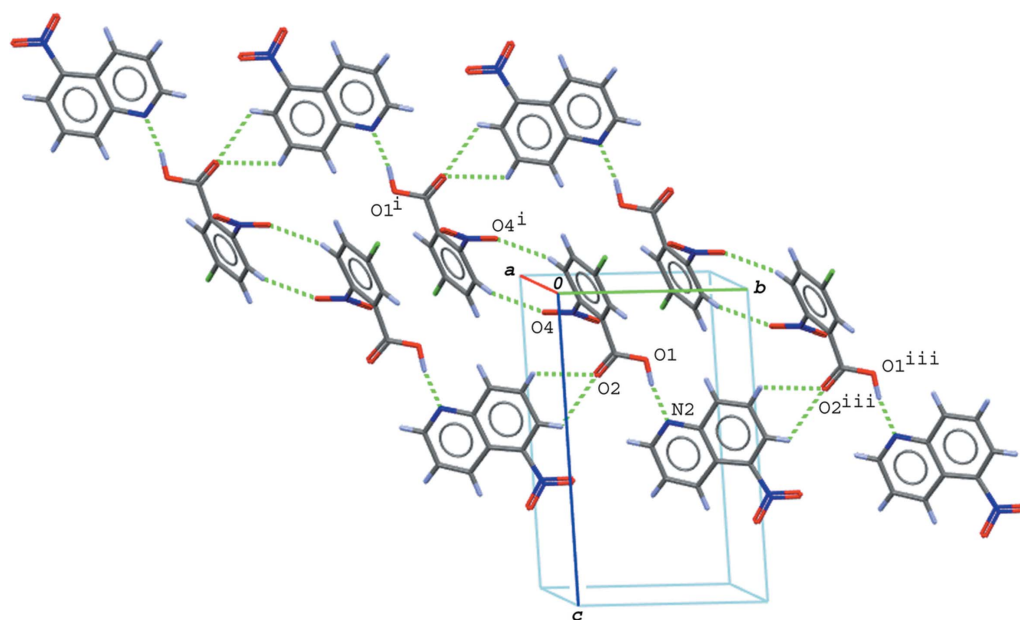


Figure 4

A packing diagram of (II), showing the wide ribbon structure running along $[1\bar{1}0]$ formed by O—H···N and C—H···O hydrogen bonds (green dashed lines). [Symmetry codes: (i) $-x + 2, -y, -z$; (iii) $x - 1, y + 1, z$.]

3.94 (17) and 7.5 (5)°, respectively, with the benzene ring (C1–C6) and the carboxy group (O1/C7/O2). In the acid molecule, the benzene ring makes dihedral angles of 4.3 (5) and 2.5 (5)°, respectively, with the carboxy group and the nitro group (O3/N1/O4), while in the base molecule, the quinoline ring system and the attached nitro group (O5/N3/O6) are somewhat twisted with a dihedral angle of 36.2 (5)°.

The molecular structure of (II) is shown in Fig. 2. Similar to (I), the acid and base molecules are held together by an O–H···N hydrogen bond (Table 2). In the acid–base unit, the quinoline ring system and the hydrogen-bonded carboxy group are almost coplanar, with a dihedral angle of 2.9 (2)°, while the quinoline ring system and the benzene ring of the acid are twisted with respect to each other by a dihedral angle of 37.37 (6)°. In the acid molecule, the benzene ring makes dihedral angles of 40.3 (2) and 47.12 (19)°, respectively, with the carboxy and nitro groups. In the base molecule, the dihedral angle between the quinoline ring system and the attached nitro group is 11.3 (2)°.

3. Supramolecular features

In the crystal of (I), the hydrogen-bonded acid–base units are linked by a C–H···O hydrogen bond (C13–H13···O4ⁱⁱ; symmetry code as in Table 1), forming a tape structure along

[1 $\bar{2}$ 0]. The tapes are stacked into a layer parallel to the *ab* plane (Fig. 3) *via* N–O··· π contacts (N3–O5···Cg3ⁱⁱⁱ and N3–O5···Cg4ⁱⁱⁱ; Table 1) between the nitro group of the base and the quinoline ring system; Cg3 and Cg4 are the centroids of the C11–C16 ring and the N2/C8–C16 ring system of the base molecule, respectively. The layers are further linked by other C–H···O hydrogen bonds (C8–H8···O2ⁱ and C9–H9···O2ⁱ; Table 1), forming a three-dimensional network.

In the crystal of (II), the hydrogen-bonded acid–base units are linked into a wide ribbon structure running along [1 $\bar{1}$ 0] (Fig. 4) *via* C–H···O hydrogen bonds (C3–H3···O4ⁱ, C13–H13···O2ⁱⁱⁱ and C14–H14···O2ⁱⁱⁱ; symmetry codes as in Table 2); the mean plane of the non-H atoms in the ribbon is parallel to (773). The ribbons are further linked *via* another C–H···O hydrogen bond (C10–H10···O3ⁱⁱ; Table 2), forming a layer parallel to (110). Between the layers, weak π – π interactions are observed; the centroid–centroid distances are 3.7080 (10) and 3.7543 (9) Å, respectively, for Cg2···Cg2^{iv} and Cg2···Cg4^{vi}, where Cg2 and Cg4 are the centroids of the N2/C8–C11/C16 ring and the N2/C8–C16 ring system of the base molecule, respectively [symmetry code: (iv) $-x, -y + 1, -z + 1$].

Hirshfeld surfaces for the 5-nitroquinoline molecules of (I) and (II), mapped over shape index and d_{norm} (Turner *et al.*, 2017; McKinnon *et al.*, 2004, 2007), are shown in Figs. 5 and 6.

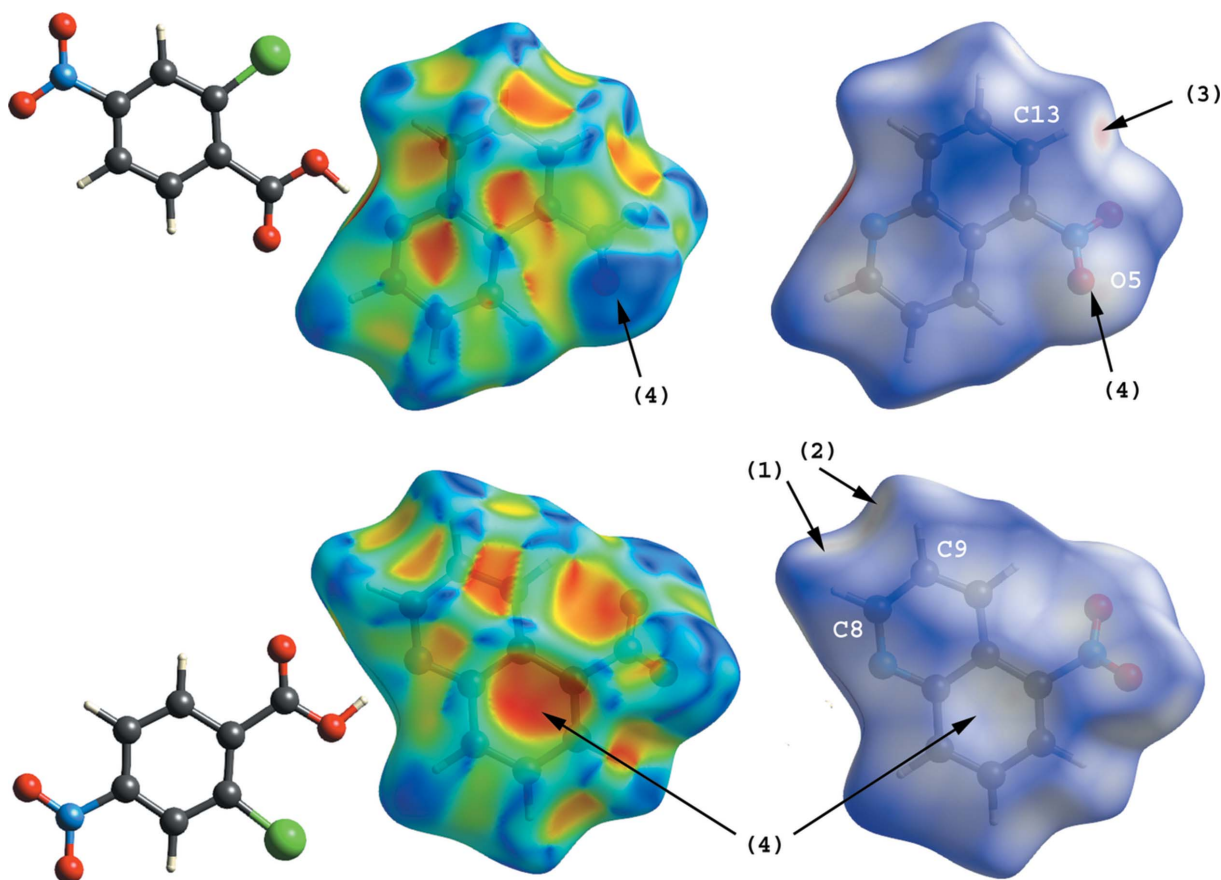


Figure 5
Hirshfeld surfaces [front (top) and back (bottom) views] for the 5-nitroquinoline molecule of (I) mapped over shape index and d_{norm} , indicating the C–H···O [arrows (1)–(3)] and N–O··· π [arrows (4)] interactions.

The three C—H···O interactions in (I) (C8—H8···O2ⁱ, C9—H9···O2^j and C13—H13···O4ⁱⁱ; Table 1) are viewed as faint-red spots on the d_{norm} surfaces [arrows (1)–(3); Fig. 5]. In addition to these interactions, the N—O··· π contacts (N3—O5···Cg3ⁱⁱⁱ and N3—O5···Cg4ⁱⁱⁱ; Table 1) are shown as broad blue and red regions, respectively, in the front and back views of shape-index surfaces [arrows (4)]. The three C—H···O interactions in (II) (C10—H10···O3ⁱⁱ, C13—H13···O2ⁱⁱⁱ and C14—H14···O2ⁱⁱⁱ; Table 2) are also represented as faint-red spots on the d_{norm} surfaces [arrows (1)–(3); Fig. 6]. By contrast with the shape-index surfaces of (I), π – π interactions between the quinoline ring systems of inversion-related molecules [$Cg2$ ··· $Cg2^{\text{iv}}$ and $Cg2$ ··· $Cg4^{\text{vi}}$; symmetry code: (iv) $-x, -y + 1, -z + 1$] are indicated by blue and red triangles on the shape-index surface [arrow (4) in the front view of (II)].

4. Database survey

A search of the Cambridge Structural Database (Version 5.40, last update August 2019; Groom *et al.*, 2016) for organic cocrystals/salts of 5-nitroquinoline with carboxylic acid deri-

vatives gave five structures, namely, 3-aminobenzoic acid–5-nitroquinoline (1/1) (refcode PANYIM; Lynch *et al.*, 1997), 4-aminobenzoic acid–5-nitroquinoline (1/2) (PANZEJ; Lynch *et al.*, 1997), indole-2-carboxylic acid–5-nitroquinoline (1/2) (GISGUK; Lynch *et al.*, 1998), indole-3-acetic acid–5-nitroquinoline (1/2) (GISHAR; Lynch *et al.*, 1998) and (2,4,5-trichlorophenoxy)acetic acid–5-nitroquinoline (1/1) (XAPWOA; Lynch *et al.*, 1999). In these compounds, the dihedral angles between the quinoline ring system and the attached nitro group vary in the wide range 2.2 (4)–32.9 (4)°, which implies that the orientation of the nitro group is mainly affected by intermolecular interactions.

A search for organic cocrystals/salts of 2-chloro-4-nitrobenzoic acid with base molecules gave 60 structures, while for organic cocrystals/salts of 5-chloro-2-nitrobenzoic acid with base molecules, five compounds were reported. Limiting the search to quinoline derivatives of these compounds gave three compounds, namely, 2-chloro-4-nitrobenzoic acid–quinoline (1/1) (YAGFAP; Gotoh & Ishida, 2011*b*), 8-hydroxyquinolinium 2-chloro-4-nitrobenzoate (WOPDEM; Babu & Chandrasekaran, 2014) and 5-chloro-2-nitrobenzoic acid–quinoline (1/1) (AJIXAT; Gotoh & Ishida, 2009).

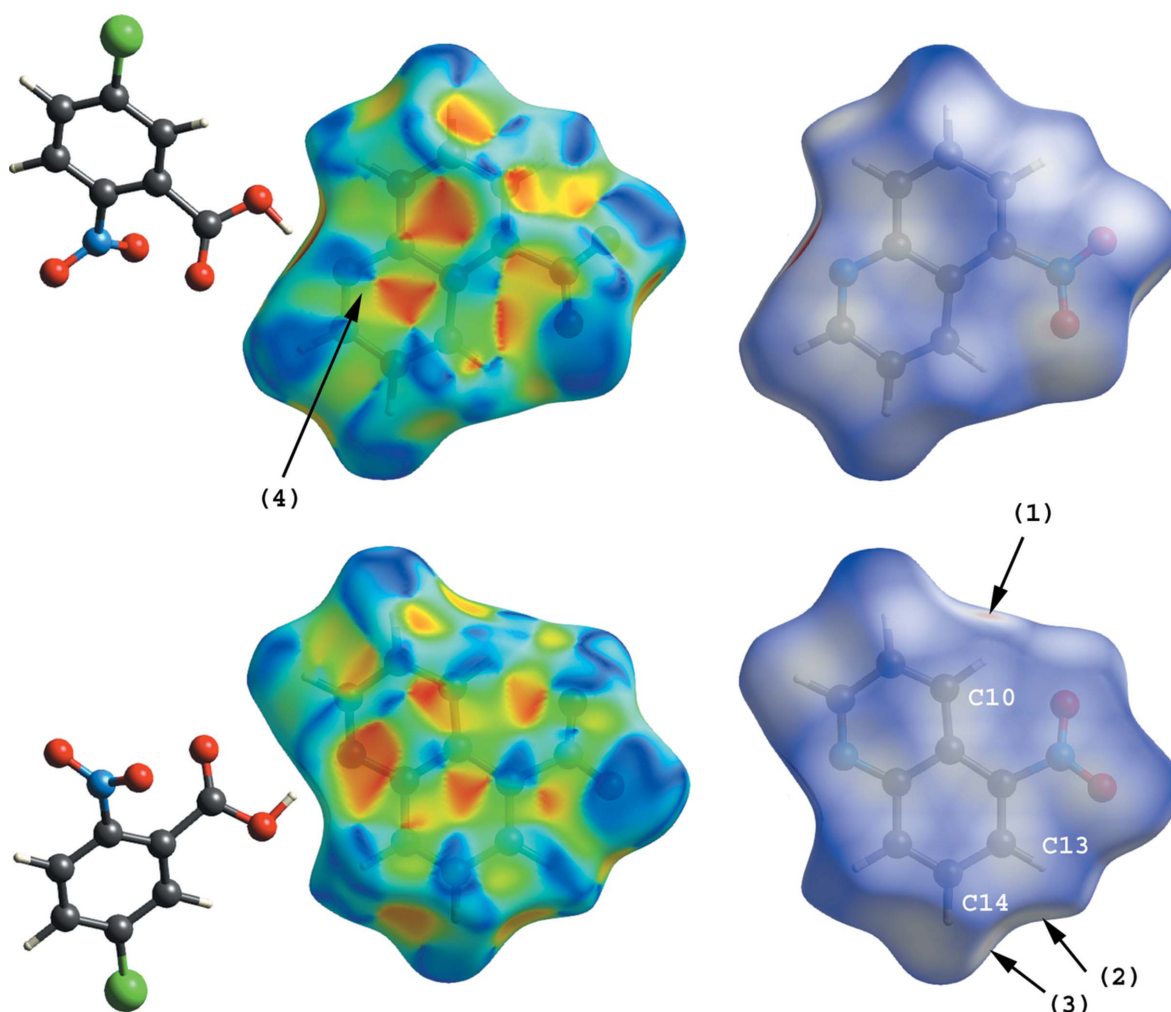


Figure 6

Hirshfeld surfaces [front (top) and back (bottom) views] for the 5-nitroquinoline molecule of (II) mapped over shape index and d_{norm} , indicating the C—H···O [arrows (1)–(3)] and π – π [arrow (4)] interactions.

5. Synthesis and crystallization

Crystals of compounds (I) and (II) were obtained by slow evaporation from acetonitrile solutions of 5-nitroquinoline with chloronitrobenzoic acids in a 1:1 molar ratio at room temperature [80 ml acetonitrile solution of 5-nitroquinoline (0.117 g) and 2-chloro-4-nitrobenzoic acid (0.135 g) for (I), and 50 ml acetonitrile solution of 5-nitroquinoline (0.099 g) and 5-chloro-2-nitrobenzoic acid (0.112 g) for (II)].

6. Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 3. All H atoms in compounds (I) and (II) were found in difference Fourier maps. H atoms on O atoms in (I) and (II) were refined freely, with distances of O1–H1 = 1.02 (8) Å in (I) and O1–H1 = 0.99 (4) Å in (II). Other H atoms were positioned geometrically (C–H = 0.95 Å) and treated as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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supporting information

Acta Cryst. (2019). E75, 1694-1699 [https://doi.org/10.1107/S2056989019013896]

Crystal structures of the two isomeric hydrogen-bonded cocrystals 2-chloro-4-nitrobenzoic acid–5-nitroquinoline (1/1) and 5-chloro-2-nitrobenzoic acid–5-nitroquinoline (1/1)

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Computing details

For both structures, data collection: *PROCESS-AUTO* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 2006); data reduction: *PROCESS-AUTO* (Rigaku, 2006); program(s) used to solve structure: *SHELXT2018* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2018) and *PLATON* (Spek, 2015).

2-Chloro-4-nitrobenzoic acid–5-nitroquinoline (I)

Crystal data

$C_7H_4ClNO_4 \cdot C_9H_6N_2O_2$
 $M_r = 375.72$
 Monoclinic, $P2_1$
 $a = 12.8265$ (13) Å
 $b = 4.7699$ (5) Å
 $c = 13.5033$ (16) Å
 $\beta = 109.713$ (3)°
 $V = 777.73$ (15) Å³
 $Z = 2$

$F(000) = 384.00$
 $D_x = 1.604$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
 Cell parameters from 11483 reflections
 $\theta = 3.1$ – 30.0°
 $\mu = 0.29$ mm⁻¹
 $T = 190$ K
 Block, colorless
 $0.37 \times 0.18 \times 0.10$ mm

Data collection

Rigaku R-AXIS RAPID
 diffractometer
 Detector resolution: 10.000 pixels mm⁻¹
 ω scans
 Absorption correction: numerical
 (NUMABS; Higashi, 1999)
 $T_{\min} = 0.913$, $T_{\max} = 0.972$
 14435 measured reflections

4168 independent reflections
 2859 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.058$
 $\theta_{\max} = 30.0^\circ$, $\theta_{\min} = 3.1^\circ$
 $h = -17 \rightarrow 18$
 $k = -6 \rightarrow 6$
 $l = -18 \rightarrow 18$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.056$
 $wR(F^2) = 0.169$
 $S = 1.05$
 4168 reflections
 239 parameters

1 restraint
 Primary atom site location: structure-invariant
 direct methods
 Secondary atom site location: difference Fourier
 map
 Hydrogen site location: mixed

H atoms treated by a mixture of independent

and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0939P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.64 \text{ e } \text{\AA}^{-3}$$

Absolute structure: Flack x determined using

898 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)

Absolute structure parameter: 0.01 (6)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.57519 (8)	0.0684 (3)	0.43612 (8)	0.0493 (3)
O1	0.5077 (3)	0.4634 (8)	0.2687 (3)	0.0477 (8)
O2	0.5751 (3)	0.4867 (9)	0.1386 (3)	0.0558 (10)
O3	0.9097 (3)	-0.5701 (8)	0.4815 (3)	0.0521 (8)
O4	0.9774 (2)	-0.4811 (7)	0.3586 (3)	0.0484 (8)
O5	0.0470 (2)	1.5716 (7)	0.0857 (3)	0.0485 (7)
O6	-0.0635 (2)	1.3007 (9)	0.1321 (3)	0.0555 (9)
N1	0.9100 (3)	-0.4421 (8)	0.4027 (3)	0.0383 (7)
N2	0.3733 (3)	0.8494 (8)	0.1655 (3)	0.0372 (8)
N3	0.0279 (3)	1.3624 (8)	0.1297 (3)	0.0410 (8)
C1	0.6593 (3)	0.1676 (9)	0.2761 (3)	0.0338 (8)
C2	0.6664 (3)	0.0245 (9)	0.3678 (3)	0.0369 (9)
C3	0.7492 (3)	-0.1771 (10)	0.4099 (3)	0.0381 (9)
H3	0.753753	-0.276100	0.472305	0.046*
C4	0.8238 (3)	-0.2282 (9)	0.3586 (3)	0.0365 (8)
C5	0.8196 (3)	-0.0934 (10)	0.2676 (3)	0.0381 (9)
H5	0.871190	-0.135533	0.233150	0.046*
C6	0.7376 (3)	0.1061 (9)	0.2273 (3)	0.0371 (9)
H6	0.734210	0.204031	0.165071	0.045*
C7	0.5754 (3)	0.3898 (9)	0.2214 (3)	0.0364 (9)
C8	0.3804 (3)	0.9609 (11)	0.0786 (3)	0.0411 (10)
H8	0.438654	0.903116	0.054610	0.049*
C9	0.3047 (4)	1.1621 (10)	0.0206 (3)	0.0424 (10)
H9	0.313962	1.243052	-0.040174	0.051*
C10	0.2177 (3)	1.2428 (10)	0.0506 (3)	0.0389 (9)
H10	0.165082	1.375120	0.010283	0.047*
C11	0.2075 (3)	1.1243 (8)	0.1438 (3)	0.0341 (9)
C12	0.1202 (3)	1.1733 (9)	0.1847 (3)	0.0371 (9)
C13	0.1160 (3)	1.0509 (11)	0.2741 (3)	0.0402 (9)
H13	0.057188	1.093775	0.299480	0.048*
C14	0.1991 (4)	0.8605 (10)	0.3290 (3)	0.0435 (10)
H14	0.196326	0.774460	0.391516	0.052*
C15	0.2838 (3)	0.7987 (10)	0.2925 (3)	0.0411 (10)

H15	0.339701	0.669393	0.329616	0.049*
C16	0.2884 (3)	0.9272 (9)	0.1997 (3)	0.0343 (8)
H1	0.463 (5)	0.632 (17)	0.231 (5)	0.09 (2)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0495 (5)	0.0641 (7)	0.0462 (5)	0.0116 (6)	0.0317 (4)	0.0062 (5)
O1	0.0504 (17)	0.0543 (19)	0.0481 (18)	0.0154 (16)	0.0296 (14)	0.0074 (15)
O2	0.0569 (18)	0.072 (3)	0.0509 (18)	0.0215 (19)	0.0349 (16)	0.0194 (17)
O3	0.0518 (17)	0.053 (2)	0.058 (2)	0.0071 (17)	0.0268 (15)	0.0135 (17)
O4	0.0453 (15)	0.051 (2)	0.0562 (18)	0.0121 (16)	0.0265 (14)	-0.0026 (15)
O5	0.0488 (16)	0.0386 (16)	0.0605 (18)	0.0045 (17)	0.0214 (14)	0.0071 (17)
O6	0.0395 (16)	0.075 (3)	0.059 (2)	0.0106 (18)	0.0262 (14)	0.0093 (19)
N1	0.0357 (15)	0.0351 (17)	0.0474 (18)	0.0017 (17)	0.0183 (13)	-0.0015 (17)
N2	0.0367 (16)	0.0413 (19)	0.0407 (18)	0.0012 (16)	0.0221 (14)	-0.0009 (15)
N3	0.0418 (18)	0.044 (2)	0.0441 (19)	0.0080 (17)	0.0230 (16)	-0.0009 (16)
C1	0.0354 (19)	0.0340 (19)	0.0375 (19)	-0.0036 (17)	0.0196 (16)	-0.0050 (16)
C2	0.0375 (17)	0.042 (2)	0.0383 (19)	-0.0025 (19)	0.0218 (15)	-0.0042 (18)
C3	0.040 (2)	0.040 (2)	0.039 (2)	0.0023 (19)	0.0194 (16)	0.0000 (18)
C4	0.0366 (19)	0.033 (2)	0.043 (2)	0.0024 (18)	0.0178 (16)	-0.0027 (17)
C5	0.0365 (19)	0.042 (2)	0.043 (2)	0.0039 (18)	0.0229 (17)	-0.0003 (18)
C6	0.0378 (19)	0.043 (2)	0.0368 (18)	-0.0002 (19)	0.0206 (16)	-0.0005 (18)
C7	0.0346 (18)	0.039 (2)	0.041 (2)	0.0002 (18)	0.0197 (16)	-0.0029 (17)
C8	0.0389 (19)	0.050 (2)	0.042 (2)	0.001 (2)	0.0235 (18)	-0.0018 (19)
C9	0.045 (2)	0.051 (3)	0.039 (2)	0.000 (2)	0.0238 (18)	0.0054 (18)
C10	0.041 (2)	0.042 (2)	0.037 (2)	-0.0007 (19)	0.0179 (16)	0.0021 (18)
C11	0.0347 (18)	0.036 (2)	0.0365 (18)	-0.0015 (17)	0.0181 (15)	-0.0025 (16)
C12	0.036 (2)	0.037 (2)	0.043 (2)	0.0049 (17)	0.0197 (17)	-0.0022 (17)
C13	0.0387 (18)	0.046 (2)	0.044 (2)	0.002 (2)	0.0254 (16)	-0.004 (2)
C14	0.045 (2)	0.053 (3)	0.041 (2)	0.003 (2)	0.0243 (17)	0.002 (2)
C15	0.041 (2)	0.047 (2)	0.042 (2)	0.009 (2)	0.0223 (17)	0.007 (2)
C16	0.0344 (17)	0.036 (2)	0.0374 (19)	0.0017 (17)	0.0187 (15)	0.0009 (16)

Geometric parameters (Å, °)

C11—C2	1.729 (4)	C5—C6	1.386 (6)
O1—C7	1.288 (5)	C5—H5	0.9500
O1—H1	1.02 (8)	C6—H6	0.9500
O2—C7	1.209 (5)	C8—C9	1.402 (7)
O3—N1	1.228 (5)	C8—H8	0.9500
O4—N1	1.218 (4)	C9—C10	1.365 (5)
O5—N3	1.228 (5)	C9—H9	0.9500
O6—N3	1.220 (4)	C10—C11	1.425 (5)
N1—C4	1.474 (5)	C10—H10	0.9500
N2—C8	1.320 (5)	C11—C16	1.415 (6)
N2—C16	1.370 (4)	C11—C12	1.425 (5)
N3—C12	1.474 (5)	C12—C13	1.359 (6)

C1—C2	1.390 (6)	C13—C14	1.406 (6)
C1—C6	1.405 (5)	C13—H13	0.9500
C1—C7	1.514 (6)	C14—C15	1.369 (5)
C2—C3	1.403 (6)	C14—H14	0.9500
C3—C4	1.380 (5)	C15—C16	1.413 (5)
C3—H3	0.9500	C15—H15	0.9500
C4—C5	1.372 (6)		
C7—O1—H1	109 (4)	O1—C7—C1	115.9 (4)
O4—N1—O3	123.9 (4)	N2—C8—C9	122.0 (4)
O4—N1—C4	117.9 (4)	N2—C8—H8	119.0
O3—N1—C4	118.2 (3)	C9—C8—H8	119.0
C8—N2—C16	119.5 (4)	C10—C9—C8	120.6 (4)
O6—N3—O5	124.0 (4)	C10—C9—H9	119.7
O6—N3—C12	117.1 (4)	C8—C9—H9	119.7
O5—N3—C12	118.9 (3)	C9—C10—C11	118.6 (4)
C2—C1—C6	118.2 (4)	C9—C10—H10	120.7
C2—C1—C7	126.9 (3)	C11—C10—H10	120.7
C6—C1—C7	114.8 (3)	C16—C11—C12	115.6 (3)
C1—C2—C3	120.7 (3)	C16—C11—C10	117.8 (3)
C1—C2—C11	124.3 (3)	C12—C11—C10	126.5 (4)
C3—C2—C11	115.0 (3)	C13—C12—C11	123.1 (4)
C4—C3—C2	118.4 (4)	C13—C12—N3	116.4 (3)
C4—C3—H3	120.8	C11—C12—N3	120.5 (4)
C2—C3—H3	120.8	C12—C13—C14	119.7 (3)
C5—C4—C3	122.9 (4)	C12—C13—H13	120.1
C5—C4—N1	118.9 (3)	C14—C13—H13	120.1
C3—C4—N1	118.2 (4)	C15—C14—C13	120.2 (4)
C4—C5—C6	117.9 (3)	C15—C14—H14	119.9
C4—C5—H5	121.0	C13—C14—H14	119.9
C6—C5—H5	121.0	C14—C15—C16	120.0 (4)
C5—C6—C1	121.8 (4)	C14—C15—H15	120.0
C5—C6—H6	119.1	C16—C15—H15	120.0
C1—C6—H6	119.1	N2—C16—C15	117.2 (4)
O2—C7—O1	124.2 (4)	N2—C16—C11	121.5 (4)
O2—C7—C1	119.9 (4)	C15—C16—C11	121.3 (3)
C6—C1—C2—C3	-0.4 (6)	C8—C9—C10—C11	1.8 (7)
C7—C1—C2—C3	-179.9 (4)	C9—C10—C11—C16	-0.4 (6)
C6—C1—C2—C11	-178.5 (3)	C9—C10—C11—C12	-177.1 (4)
C7—C1—C2—C11	2.1 (6)	C16—C11—C12—C13	2.9 (6)
C1—C2—C3—C4	0.5 (6)	C10—C11—C12—C13	179.7 (4)
C11—C2—C3—C4	178.7 (3)	C16—C11—C12—N3	-176.6 (4)
C2—C3—C4—C5	-1.0 (7)	C10—C11—C12—N3	0.2 (6)
C2—C3—C4—N1	-179.4 (4)	O6—N3—C12—C13	-34.6 (6)
O4—N1—C4—C5	3.3 (6)	O5—N3—C12—C13	144.6 (4)
O3—N1—C4—C5	-176.7 (4)	O6—N3—C12—C11	144.9 (4)
O4—N1—C4—C3	-178.1 (4)	O5—N3—C12—C11	-35.9 (6)

O3—N1—C4—C3	1.8 (6)	C11—C12—C13—C14	-1.7 (7)
C3—C4—C5—C6	1.3 (7)	N3—C12—C13—C14	177.8 (4)
N1—C4—C5—C6	179.7 (4)	C12—C13—C14—C15	0.0 (7)
C4—C5—C6—C1	-1.2 (6)	C13—C14—C15—C16	0.2 (7)
C2—C1—C6—C5	0.8 (6)	C8—N2—C16—C15	179.2 (4)
C7—C1—C6—C5	-179.7 (4)	C8—N2—C16—C11	0.2 (6)
C2—C1—C7—O2	-176.0 (4)	C14—C15—C16—N2	-177.9 (4)
C6—C1—C7—O2	4.5 (6)	C14—C15—C16—C11	1.1 (7)
C2—C1—C7—O1	4.2 (6)	C12—C11—C16—N2	176.4 (4)
C6—C1—C7—O1	-175.3 (4)	C10—C11—C16—N2	-0.7 (6)
C16—N2—C8—C9	1.3 (7)	C12—C11—C16—C15	-2.6 (6)
N2—C8—C9—C10	-2.4 (7)	C10—C11—C16—C15	-179.6 (4)

Hydrogen-bond geometry (Å, °)

Cg3 and Cg4 are the centroids of the C11–C16 ring and the N2/C8–C16 ring system, respectively.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1...N2	1.02 (8)	1.58 (7)	2.585 (5)	168 (7)
C8—H8...O2 ⁱ	0.95	2.59	3.174 (6)	120
C9—H9...O2 ⁱ	0.95	2.56	3.152 (6)	120
C13—H13...O4 ⁱⁱ	0.95	2.52	3.289 (6)	138
N3—O5...Cg3 ⁱⁱⁱ	1.23 (1)	3.06 (1)	3.724 (4)	113 (1)
N3—O5...Cg4 ⁱⁱⁱ	1.23 (1)	3.25 (1)	4.118 (4)	128 (1)

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

5-Chloro-2-nitrobenzoic acid–5-nitroquinoline (1/1) (II)

Crystal data

C₇H₄ClNO₄·C₉H₆N₂O₂

M_r = 375.72

Triclinic, *P*1̄

a = 7.6682 (6) Å

b = 8.6515 (8) Å

c = 12.8609 (10) Å

α = 79.170 (3)°

β = 78.968 (2)°

γ = 70.394 (3)°

V = 781.80 (11) Å³

Z = 2

F(000) = 384.00

D_x = 1.596 Mg m⁻³

Mo *K*α radiation, λ = 0.71075 Å

Cell parameters from 7062 reflections

θ = 3.1–30.1°

μ = 0.29 mm⁻¹

T = 190 K

Block, colorless

0.26 × 0.20 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID
diffractometer

Detector resolution: 10.000 pixels mm⁻¹

ω scans

Absorption correction: numerical
(NUMABS; Higashi, 1999)

T_{min} = 0.933, *T_{max}* = 0.950

9772 measured reflections

4502 independent reflections

3075 reflections with *I* > 2σ(*I*)

R_{int} = 0.055

θ_{\max} = 30.0°, θ_{\min} = 3.1°

h = -10→10

k = -12→12

l = -18→16

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.148$

$S = 1.09$

4502 reflections

239 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.077P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.39 \text{ e } \text{\AA}^{-3}$

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. Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

$_reflns_Friedel_fraction$ is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.

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

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
Cl1	0.14420 (7)	0.28783 (7)	-0.10243 (4)	0.05199 (18)
O1	0.27021 (17)	0.49296 (15)	0.23397 (9)	0.0398 (3)
O2	0.49601 (18)	0.27221 (17)	0.29240 (9)	0.0464 (3)
O3	0.7904 (2)	0.35306 (18)	0.13902 (11)	0.0517 (4)
O4	0.91612 (19)	0.09724 (19)	0.11445 (12)	0.0560 (4)
O5	-0.2211 (2)	0.9235 (2)	0.73000 (11)	0.0588 (4)
O6	-0.3859 (2)	1.13276 (19)	0.63614 (12)	0.0585 (4)
N1	0.78959 (19)	0.22747 (19)	0.10917 (11)	0.0375 (3)
N2	0.18718 (18)	0.57290 (17)	0.42980 (10)	0.0304 (3)
N3	-0.2703 (2)	0.99626 (19)	0.64474 (12)	0.0363 (3)
C1	0.4473 (2)	0.31055 (18)	0.11065 (11)	0.0280 (3)
C2	0.6260 (2)	0.2358 (2)	0.06195 (12)	0.0311 (3)
C3	0.6607 (3)	0.1738 (2)	-0.03429 (13)	0.0394 (4)
H3	0.785039	0.121041	-0.064631	0.047*
C4	0.5112 (3)	0.1900 (2)	-0.08550 (13)	0.0405 (4)
H4	0.531267	0.149424	-0.151912	0.049*
C5	0.3327 (2)	0.2660 (2)	-0.03861 (12)	0.0347 (4)
C6	0.2973 (2)	0.3264 (2)	0.05903 (12)	0.0322 (3)
H6	0.172692	0.377559	0.089801	0.039*
C7	0.4089 (2)	0.3576 (2)	0.22188 (12)	0.0289 (3)
C8	0.2766 (2)	0.4942 (2)	0.51114 (13)	0.0338 (4)
H8	0.379851	0.397342	0.501163	0.041*
C9	0.2254 (2)	0.5479 (2)	0.61268 (13)	0.0360 (4)
H9	0.295494	0.488936	0.669132	0.043*
C10	0.0752 (2)	0.6842 (2)	0.62990 (12)	0.0329 (4)

H10	0.039659	0.720138	0.698459	0.039*
C11	-0.0277 (2)	0.77237 (19)	0.54485 (11)	0.0262 (3)
C12	-0.1866 (2)	0.9174 (2)	0.54633 (12)	0.0287 (3)
C13	-0.2716 (2)	0.9935 (2)	0.45823 (13)	0.0335 (3)
H13	-0.376955	1.090140	0.462933	0.040*
C14	-0.2037 (2)	0.9294 (2)	0.36000 (13)	0.0364 (4)
H14	-0.264213	0.981948	0.298918	0.044*
C15	-0.0520 (2)	0.7928 (2)	0.35311 (12)	0.0335 (4)
H15	-0.005289	0.751029	0.286601	0.040*
C16	0.0378 (2)	0.71153 (19)	0.44377 (11)	0.0269 (3)
H1	0.249 (4)	0.510 (4)	0.310 (3)	0.097 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0591 (3)	0.0735 (4)	0.0357 (3)	-0.0300 (3)	-0.0154 (2)	-0.0106 (2)
O1	0.0383 (7)	0.0413 (7)	0.0295 (6)	0.0079 (5)	-0.0075 (5)	-0.0150 (5)
O2	0.0500 (8)	0.0468 (8)	0.0289 (6)	0.0086 (6)	-0.0146 (5)	-0.0075 (5)
O3	0.0544 (8)	0.0521 (9)	0.0544 (8)	-0.0177 (7)	-0.0210 (7)	-0.0056 (7)
O4	0.0337 (7)	0.0574 (10)	0.0559 (8)	0.0116 (6)	-0.0050 (6)	-0.0061 (7)
O5	0.0689 (10)	0.0644 (10)	0.0325 (7)	-0.0043 (8)	0.0003 (7)	-0.0192 (7)
O6	0.0579 (9)	0.0479 (9)	0.0567 (9)	0.0053 (7)	-0.0009 (7)	-0.0234 (7)
N1	0.0296 (7)	0.0450 (9)	0.0289 (7)	-0.0034 (6)	-0.0018 (5)	-0.0007 (6)
N2	0.0294 (6)	0.0313 (7)	0.0293 (6)	-0.0064 (5)	-0.0030 (5)	-0.0079 (5)
N3	0.0347 (8)	0.0400 (8)	0.0355 (7)	-0.0129 (6)	0.0037 (6)	-0.0147 (6)
C1	0.0310 (8)	0.0252 (7)	0.0227 (7)	-0.0023 (6)	-0.0029 (6)	-0.0038 (6)
C2	0.0302 (8)	0.0287 (8)	0.0288 (7)	-0.0030 (6)	-0.0037 (6)	-0.0022 (6)
C3	0.0409 (9)	0.0378 (9)	0.0310 (8)	-0.0029 (7)	0.0048 (7)	-0.0111 (7)
C4	0.0538 (11)	0.0396 (10)	0.0275 (8)	-0.0120 (8)	-0.0001 (7)	-0.0130 (7)
C5	0.0455 (10)	0.0364 (9)	0.0252 (7)	-0.0145 (7)	-0.0090 (7)	-0.0040 (7)
C6	0.0324 (8)	0.0343 (8)	0.0262 (7)	-0.0045 (7)	-0.0042 (6)	-0.0057 (6)
C7	0.0285 (7)	0.0313 (8)	0.0244 (7)	-0.0035 (6)	-0.0052 (6)	-0.0067 (6)
C8	0.0298 (8)	0.0339 (9)	0.0371 (8)	-0.0069 (7)	-0.0079 (6)	-0.0054 (7)
C9	0.0365 (9)	0.0405 (9)	0.0321 (8)	-0.0107 (7)	-0.0129 (7)	-0.0016 (7)
C10	0.0356 (8)	0.0410 (9)	0.0251 (7)	-0.0134 (7)	-0.0057 (6)	-0.0078 (7)
C11	0.0276 (7)	0.0294 (8)	0.0242 (7)	-0.0121 (6)	-0.0023 (5)	-0.0051 (6)
C12	0.0279 (7)	0.0305 (8)	0.0283 (7)	-0.0109 (6)	0.0021 (6)	-0.0080 (6)
C13	0.0286 (8)	0.0301 (8)	0.0387 (9)	-0.0072 (6)	-0.0023 (6)	-0.0033 (7)
C14	0.0355 (9)	0.0393 (9)	0.0305 (8)	-0.0070 (7)	-0.0089 (7)	0.0007 (7)
C15	0.0368 (9)	0.0382 (9)	0.0237 (7)	-0.0081 (7)	-0.0054 (6)	-0.0052 (6)
C16	0.0268 (7)	0.0298 (8)	0.0245 (7)	-0.0093 (6)	-0.0027 (6)	-0.0045 (6)

Geometric parameters (Å, °)

C11—C5	1.7351 (17)	C4—H4	0.9500
O1—C7	1.3022 (18)	C5—C6	1.395 (2)
O1—H1	1.00 (3)	C6—H6	0.9500
O2—C7	1.2098 (19)	C8—C9	1.409 (2)

O3—N1	1.2207 (19)	C8—H8	0.9500
O4—N1	1.2158 (19)	C9—C10	1.362 (2)
O5—N3	1.217 (2)	C9—H9	0.9500
O6—N3	1.216 (2)	C10—C11	1.419 (2)
N1—C2	1.470 (2)	C10—H10	0.9500
N2—C8	1.312 (2)	C11—C12	1.426 (2)
N2—C16	1.365 (2)	C11—C16	1.431 (2)
N3—C12	1.4829 (19)	C12—C13	1.362 (2)
C1—C2	1.385 (2)	C13—C14	1.411 (2)
C1—C6	1.391 (2)	C13—H13	0.9500
C1—C7	1.5085 (19)	C14—C15	1.355 (2)
C2—C3	1.385 (2)	C14—H14	0.9500
C3—C4	1.384 (3)	C15—C16	1.415 (2)
C3—H3	0.9500	C15—H15	0.9500
C4—C5	1.378 (2)		
C7—O1—H1	107.9 (18)	O1—C7—C1	113.35 (13)
O4—N1—O3	124.32 (16)	N2—C8—C9	122.56 (15)
O4—N1—C2	118.09 (15)	N2—C8—H8	118.7
O3—N1—C2	117.58 (14)	C9—C8—H8	118.7
C8—N2—C16	119.04 (13)	C10—C9—C8	119.96 (15)
O6—N3—O5	122.72 (14)	C10—C9—H9	120.0
O6—N3—C12	117.87 (15)	C8—C9—H9	120.0
O5—N3—C12	119.41 (15)	C9—C10—C11	119.64 (14)
C2—C1—C6	118.14 (13)	C9—C10—H10	120.2
C2—C1—C7	122.53 (13)	C11—C10—H10	120.2
C6—C1—C7	118.97 (13)	C10—C11—C12	128.17 (13)
C1—C2—C3	122.79 (15)	C10—C11—C16	116.46 (14)
C1—C2—N1	120.19 (13)	C12—C11—C16	115.35 (14)
C3—C2—N1	116.94 (14)	C13—C12—C11	122.78 (13)
C4—C3—C2	118.91 (16)	C13—C12—N3	115.36 (14)
C4—C3—H3	120.5	C11—C12—N3	121.86 (14)
C2—C3—H3	120.5	C12—C13—C14	120.30 (15)
C5—C4—C3	118.91 (14)	C12—C13—H13	119.9
C5—C4—H4	120.5	C14—C13—H13	119.9
C3—C4—H4	120.5	C15—C14—C13	119.77 (15)
C4—C5—C6	122.30 (15)	C15—C14—H14	120.1
C4—C5—C11	119.31 (12)	C13—C14—H14	120.1
C6—C5—C11	118.40 (13)	C14—C15—C16	120.81 (14)
C1—C6—C5	118.93 (15)	C14—C15—H15	119.6
C1—C6—H6	120.5	C16—C15—H15	119.6
C5—C6—H6	120.5	N2—C16—C15	116.71 (13)
O2—C7—O1	124.62 (13)	N2—C16—C11	122.30 (14)
O2—C7—C1	121.98 (14)	C15—C16—C11	120.99 (14)
C6—C1—C2—C3	-1.3 (3)	C8—C9—C10—C11	-0.6 (2)
C7—C1—C2—C3	171.77 (16)	C9—C10—C11—C12	-179.44 (15)
C6—C1—C2—N1	175.37 (14)	C9—C10—C11—C16	-1.2 (2)

C7—C1—C2—N1	-11.5 (2)	C10—C11—C12—C13	178.45 (16)
O4—N1—C2—C1	135.40 (16)	C16—C11—C12—C13	0.2 (2)
O3—N1—C2—C1	-45.7 (2)	C10—C11—C12—N3	-1.3 (2)
O4—N1—C2—C3	-47.7 (2)	C16—C11—C12—N3	-179.55 (13)
O3—N1—C2—C3	131.17 (17)	O6—N3—C12—C13	-11.0 (2)
C1—C2—C3—C4	1.4 (3)	O5—N3—C12—C13	169.25 (16)
N1—C2—C3—C4	-175.35 (16)	O6—N3—C12—C11	168.68 (15)
C2—C3—C4—C5	-0.6 (3)	O5—N3—C12—C11	-11.0 (2)
C3—C4—C5—C6	-0.3 (3)	C11—C12—C13—C14	0.2 (2)
C3—C4—C5—C11	179.69 (14)	N3—C12—C13—C14	179.91 (14)
C2—C1—C6—C5	0.4 (2)	C12—C13—C14—C15	-0.8 (3)
C7—C1—C6—C5	-172.98 (15)	C13—C14—C15—C16	1.1 (3)
C4—C5—C6—C1	0.4 (3)	C8—N2—C16—C15	179.18 (15)
C11—C5—C6—C1	-179.59 (12)	C8—N2—C16—C11	-1.4 (2)
C2—C1—C7—O2	-37.4 (2)	C14—C15—C16—N2	178.69 (15)
C6—C1—C7—O2	135.67 (18)	C14—C15—C16—C11	-0.7 (2)
C2—C1—C7—O1	145.23 (15)	C10—C11—C16—N2	2.2 (2)
C6—C1—C7—O1	-41.7 (2)	C12—C11—C16—N2	-179.29 (13)
C16—N2—C8—C9	-0.5 (2)	C10—C11—C16—C15	-178.39 (14)
N2—C8—C9—C10	1.5 (3)	C12—C11—C16—C15	0.1 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1...N2	0.99 (4)	1.66 (4)	2.6405 (17)	169 (3)
C3—H3...O4 ⁱ	0.95	2.49	3.408 (3)	162
C10—H10...O3 ⁱⁱ	0.95	2.54	3.254 (2)	132
C13—H13...O2 ⁱⁱⁱ	0.95	2.59	3.190 (2)	121
C14—H14...O2 ⁱⁱⁱ	0.95	2.56	3.173 (2)	122

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