

Synthesis and structure of 5-[(4-fluorobenzyl)-amino]isophthalic acid featuring O—H···O and N—H··· π interactions

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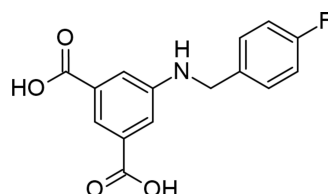
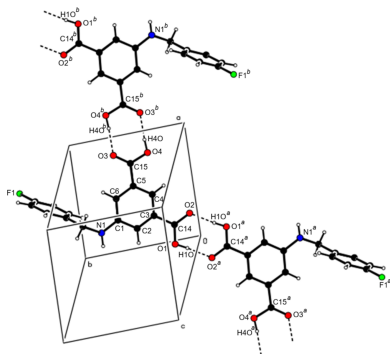
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In the title compound, C₁₅H₁₂FNO₄, the dihedral angle between the aromatic rings is 77.78 (8)°. In the crystal, the molecules are linked into zigzag ribbons propagating along the [210] direction by pairwise O—H···O hydrogen bonds through their two carboxylic acid groups to generate centrosymmetric *R*₂²(8) dimers in each case. In addition, molecules are connected *via* pairwise N—H··· π interactions between the NH groups and the fluorobenzene rings. Aromatic π – π stacking interactions and weak C—H···F and C—H···O interactions also contribute to the packing. A Hirshfeld surface analysis shows that the most important contributions to the crystal packing are from H···H (30.7%), O···H/H···O (26.1%) and C···H/H···C (20.3%) contacts.

1. Chemical context

Metal–organic frameworks (MOFs) are highly porous crystalline materials built from metal ions connected by organic ligands (Chughtai *et al.*, 2015; Liu *et al.*, 2014). The functional properties of MOFs can be improved by the design of organic ligands (carboxylates, sulfonates, phosphonates, *etc.*) and the variation of metal centres. 5-Aminoisophthalic acid and its derivatives have already been used in the synthesis and design of MOFs (Karmakar *et al.*, 2024). In order to generate an additional coordination centre and a non-covalent bond donor or acceptor site, 5-aminoisophthalic acid has been functionalized by introducing hydrazone, amide, azo, *etc.* onto its backbone (Aliyeva *et al.*, 2026). For example, halogen-bonded hydrazones of 5-amino-2,4,6-tribromoisophthalic acid were employed in the construction of new MOFs and applied in the Henry reaction of aldehydes with nitroalkanes (Gurbanov *et al.*, 2022) as well as in the coupling of CO₂ with epoxides (Aliyeva *et al.*, 2023). As a continuation of our research work in this direction, we now describe the synthesis and structure of the title compound, C₁₅H₁₂FNO₄ (**I**).



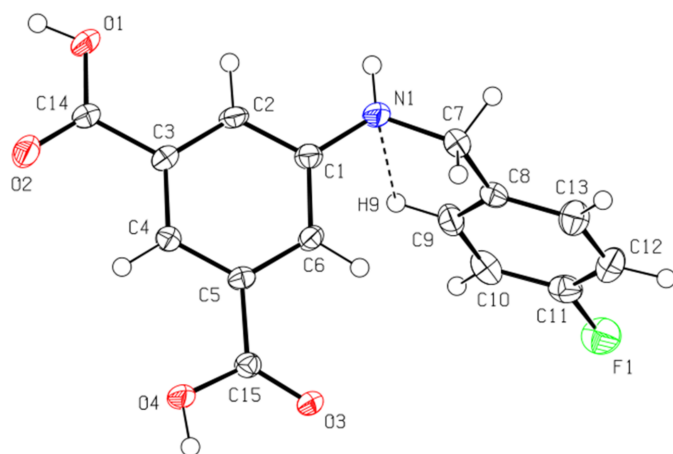


Figure 1
The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level.

2. Structural commentary

Compound (I) crystallizes in the triclinic space group $P\bar{1}$ with one molecule in the asymmetric unit (Fig. 1). The dihedral angle between the planes of the benzene-1,3-dicarboxylic acid (C1–C6) and fluorophenyl (C8–C13) rings is $77.78(8)^\circ$. The sum of the bond angles around N1 is 358.7° , implying sp^2 hybridization; the unhybridized $2p$ orbital is well aligned to interact with the π system of the C1–C6 ring, which may result in partial double-bond character for the C1–N1 bond [$1.3728(19)$ Å]. The C14/O1/O2 and C15/O3/O4 carboxylic acid groups are almost coplanar with their attached ring [dihedral angles = $3.83(19)$ and $6.7(3)^\circ$, respectively].

The C8–C7–N1 bond angle of $115.64(13)^\circ$ for the bridging methylene group deviates significantly from the nominal

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

Cg2 is the centroid of the C8–C13 benzene ring.

<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>
C9—H9...N1	0.96 (1)	2.52 (1)	2.890 (2)	103 (1)
O1—H1O...O2 ⁱ	0.86 (1)	1.77 (1)	2.6326 (16)	177 (2)
O4—H4O...O3 ⁱⁱ	0.87 (1)	1.79 (1)	2.6518 (15)	176 (2)
N1—H1N...Cg2 ⁱⁱⁱ	0.87 (1)	2.71 (2)	3.4071 (17)	139 (2)
C12—H12...F1 ^{iv}	0.96 (1)	2.46 (1)	3.2661 (19)	142 (1)
C12—H12...O3 ^v	0.96 (1)	2.65 (2)	3.298 (2)	126 (1)

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x+2, -y+1, -z$; (iii) $-x+1, -y+2, -z+1$; (iv) $-x+2, -y+3, -z+1$; (v) $-x+2, -y+2, -z+1$.

tetrahedral value of 109.5° possibly due to steric crowding. The torsion angles of the C2–C1–N1–C7, C1–N1–C7–C8 and N1–C7–C8–C13 groupings are $164.21(15)$, $89.38(19)$ and $173.68(14)^\circ$, respectively. A short intramolecular C–H...N contact (Table 1) is observed. Otherwise, all geometric parameters for (I) are normal and consistent with those of related compounds listed in the *Database survey*.

3. Supramolecular features and Hirshfeld surface analysis

In the extended structure of (I), the molecules are connected into zigzag ribbons propagating along the [210] direction by two centrosymmetric $R_2^2(8)$ dimers formed from pairwise O–H...O hydrogen bonds involving both their carboxylic acid groups (Fig. 2, Table 1). Furthermore, molecules are linked by pairwise N–H... π interactions between the NH groups and fluorobenzene rings (Fig. 3, Table 1). Simultaneously, the molecules are linked by weak π – π stacking interactions [$Cg1...Cg1^a = 3.9798(10)$ Å, shift = 2.081 Å;

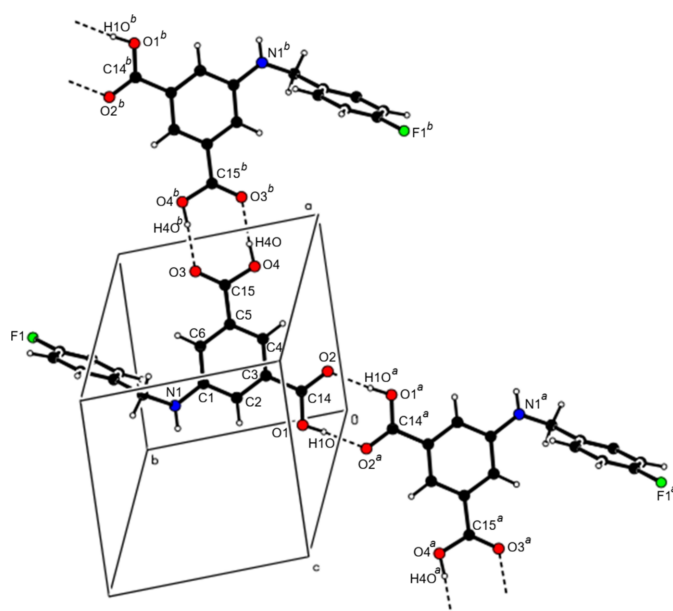


Figure 2
A partial view of the $R_2^2(8)$ motif dimers formed by pairwise O–H...O hydrogen bonds in the extended structure. Symmetry codes: (a) $-x, -y, -z$; (b) $-x+2, -y+1, -z$.

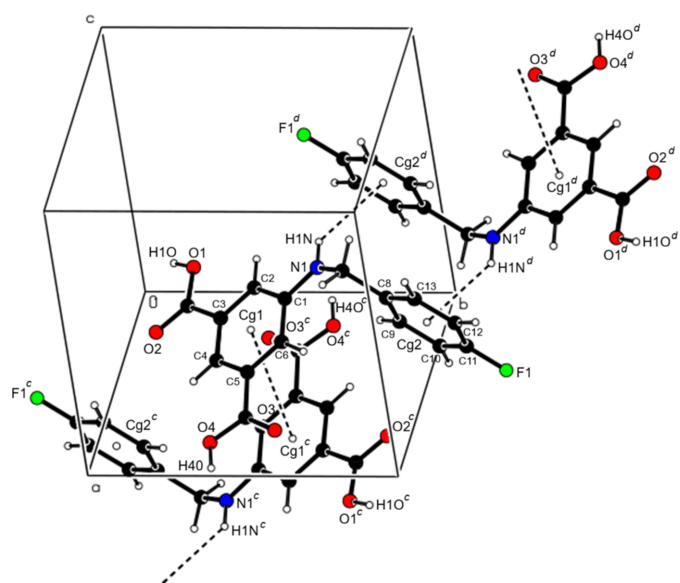
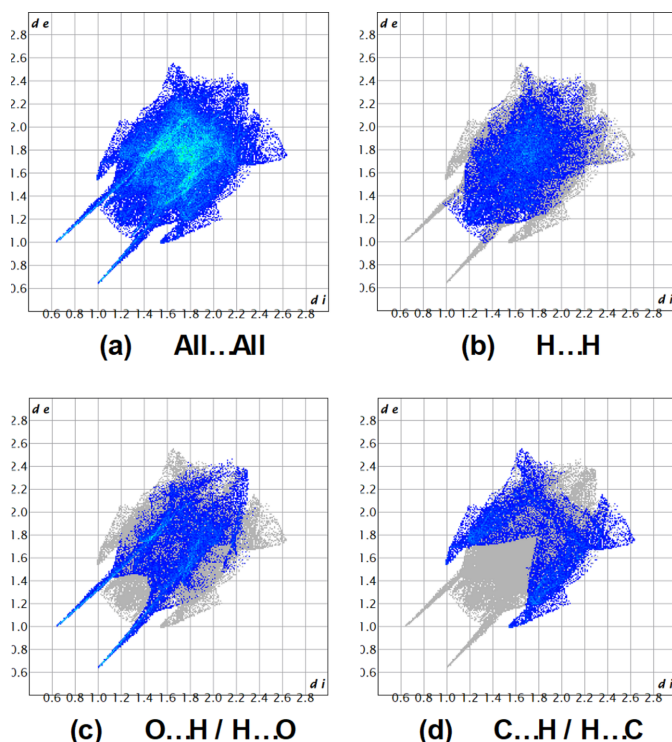


Figure 3
A partial view of the N–H... π and π – π interactions in the extended structure. Symmetry codes: (c) $-x+1, -y+1, -z$; (d) $-x+1, -y+2, -z+1$.

A Hirshfeld surface analysis was carried out to further investigate the intermolecular interactions using *Crystal Explorer 21* (Spackman *et al.*, 2021). The Hirshfeld surface mapped over d_{norm} is illustrated in Fig. 4. The red spots on the Hirshfeld surface plot indicate the directional interactions noted above. The two-dimensional fingerprint plots are shown in Fig. 5: H...H (30.7%), O...H/H...O (26.1%) and C...H/H...C (20.3%) contacts are the main contributors to the crystal packing. Minor contributions are from F...H/H...F (7.5%), O...C/C...O (4.4%), C...C (4.0%), F...C/C...F

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6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All hydrogen atoms were found from difference-Fourier maps. Hydroxyl group H atoms were refined with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$, while other H atoms were refined freely. The restraints $\text{O}—\text{H} = 0.85$ (1) Å for the OH group, $\text{N}—\text{H} = 0.86$ (1) Å for the NH group, $\text{C}—\text{H} = 0.99$ Å for the CH_2 group, and $\text{C}—\text{H} = 0.95$ Å for the CH group were applied using the DFIX command.

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The author's contributions are as follows. Conceptualization, AVG, MA and GMM; synthesis and X-ray analysis, AVG; writing (review and editing of the manuscript) AVG, AK and MA; funding acquisition, AVG; supervision, MA.

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Table 2

Experimental details.

Crystal data	
Chemical formula	$\text{C}_{15}\text{H}_{12}\text{FNO}_4$
M_r	289.26
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	150
a, b, c (Å)	8.4674 (9), 9.2193 (11), 9.2749 (11)
α, β, γ (°)	102.838 (4), 96.181 (4), 108.027 (4)
V (Å ³)	659.01 (13)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ^{−1})	0.12
Crystal size (mm)	0.35 × 0.30 × 0.21
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
$T_{\text{min}}, T_{\text{max}}$	0.954, 0.966
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8198, 2722, 2050
R_{int}	0.036
$(\sin \theta/\lambda)_{\text{max}}$ (Å ^{−1})	0.627
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.039, 0.102, 1.05
No. of reflections	2722
No. of parameters	236
No. of restraints	12
H-atom treatment	Only H-atom coordinates refined
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ^{−3})	0.24, −0.26

Computer programs: *APEX4* and *SAINT* (Bruker, 2012), *SHELXT* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

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Synthesis and structure of 5-[(4-fluorobenzyl)amino]isophthalic acid featuring O—H $\cdots$ O and N—H $\cdots\pi$ interactions

Atash V. Gurbanov, Mehmet Akkurt, Anirban Karmakar and Gizachew Mulugeta Manahelohe

Computing details

5-[[4-(4-Fluorophenyl)methyl]amino]benzene-1,3-dicarboxylic acid

Crystal data

C₁₅H₁₂FNO₄

$M_r = 289.26$

Triclinic, $P\bar{1}$

$a = 8.4674$ (9) Å

$b = 9.2193$ (11) Å

$c = 9.2749$ (11) Å

$\alpha = 102.838$ (4)°

$\beta = 96.181$ (4)°

$\gamma = 108.027$ (4)°

$V = 659.01$ (13) Å³

$Z = 2$

$F(000) = 300$

$D_x = 1.458$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2691 reflections

$\theta = 2.3\text{--}26.4^\circ$

$\mu = 0.12$ mm⁻¹

$T = 150$ K

Prism, yellow

$0.35 \times 0.30 \times 0.21$ mm

Data collection

Bruker APEXII CCD

diffractometer

φ and ω scans

Absorption correction: multi-scan

(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.954$, $T_{\max} = 0.966$

8198 measured reflections

2722 independent reflections

2050 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 26.5^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -10 \rightarrow 9$

$k = -10 \rightarrow 11$

$l = -9 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.102$

$S = 1.05$

2722 reflections

236 parameters

12 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: difference Fourier map

Only H-atom coordinates refined

$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.1305P]$

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

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

$\Delta\rho_{\max} = 0.24$ e Å⁻³

$\Delta\rho_{\min} = -0.26$ 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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.90425 (13)	1.37822 (11)	0.33763 (12)	0.0396 (3)
O1	0.06367 (14)	0.18670 (14)	0.13695 (15)	0.0393 (3)
H1O	−0.021 (2)	0.1019 (17)	0.093 (2)	0.059*
O2	0.20181 (15)	0.07050 (14)	−0.01296 (16)	0.0469 (4)
O3	0.92015 (12)	0.60399 (12)	0.11820 (12)	0.0242 (3)
O4	0.79097 (13)	0.35250 (12)	−0.01900 (13)	0.0272 (3)
H4O	0.8879 (15)	0.370 (2)	−0.048 (2)	0.041*
N1	0.49379 (17)	0.70687 (15)	0.43757 (16)	0.0280 (3)
H1N	0.4006 (16)	0.700 (2)	0.470 (2)	0.043 (6)*
C1	0.49554 (18)	0.58645 (17)	0.32082 (17)	0.0210 (3)
C2	0.34918 (19)	0.45235 (17)	0.25993 (18)	0.0213 (3)
H2	0.2474 (14)	0.4463 (18)	0.2968 (17)	0.024 (4)*
C3	0.35070 (18)	0.32787 (17)	0.14517 (17)	0.0201 (3)
C4	0.49641 (18)	0.33361 (17)	0.08617 (17)	0.0195 (3)
H4	0.4986 (18)	0.2491 (14)	0.0081 (14)	0.021 (4)*
C5	0.63955 (17)	0.46746 (16)	0.14245 (16)	0.0182 (3)
C6	0.63946 (18)	0.59342 (17)	0.25752 (17)	0.0200 (3)
H6	0.7376 (14)	0.6865 (13)	0.2898 (16)	0.017 (4)*
C7	0.6451 (2)	0.82871 (18)	0.53084 (18)	0.0255 (4)
H7A	0.7382 (16)	0.7843 (17)	0.5426 (18)	0.027 (4)*
H7B	0.623 (2)	0.8617 (19)	0.6336 (12)	0.029 (4)*
C8	0.71148 (19)	0.97471 (17)	0.47556 (17)	0.0227 (4)
C9	0.6414 (2)	0.98566 (18)	0.33749 (18)	0.0269 (4)
H9	0.5464 (16)	0.8975 (15)	0.2762 (17)	0.034 (5)*
C10	0.7055 (2)	1.12091 (19)	0.28966 (19)	0.0294 (4)
H10	0.660 (2)	1.128 (2)	0.1941 (14)	0.039 (5)*
C11	0.8393 (2)	1.24435 (18)	0.38301 (19)	0.0271 (4)
C12	0.9112 (2)	1.23975 (19)	0.5208 (2)	0.0306 (4)
H12	0.9998 (18)	1.3310 (15)	0.5851 (18)	0.042 (5)*
C13	0.8465 (2)	1.10370 (19)	0.5663 (2)	0.0295 (4)
H13	0.8931 (19)	1.0945 (19)	0.6609 (13)	0.029 (4)*
C14	0.19642 (19)	0.18422 (18)	0.08348 (18)	0.0242 (4)
C15	0.79660 (18)	0.48153 (17)	0.08001 (17)	0.0199 (3)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0492 (6)	0.0294 (5)	0.0471 (7)	0.0152 (5)	0.0171 (5)	0.0177 (5)
O1	0.0181 (6)	0.0352 (7)	0.0475 (8)	−0.0046 (5)	0.0140 (6)	−0.0065 (6)

O2	0.0265 (7)	0.0311 (7)	0.0608 (9)	−0.0037 (5)	0.0170 (6)	−0.0162 (6)
O3	0.0163 (5)	0.0229 (5)	0.0279 (6)	0.0021 (4)	0.0077 (5)	0.0014 (5)
O4	0.0176 (6)	0.0246 (6)	0.0345 (7)	0.0044 (5)	0.0115 (5)	−0.0007 (5)
N1	0.0193 (7)	0.0247 (7)	0.0337 (8)	0.0037 (6)	0.0118 (6)	−0.0019 (6)
C1	0.0198 (8)	0.0203 (7)	0.0237 (8)	0.0071 (6)	0.0070 (6)	0.0062 (6)
C2	0.0158 (8)	0.0234 (8)	0.0263 (8)	0.0059 (6)	0.0096 (6)	0.0082 (6)
C3	0.0158 (7)	0.0199 (7)	0.0235 (8)	0.0034 (6)	0.0041 (6)	0.0077 (6)
C4	0.0189 (8)	0.0188 (7)	0.0204 (8)	0.0062 (6)	0.0048 (6)	0.0041 (6)
C5	0.0152 (7)	0.0211 (7)	0.0203 (8)	0.0068 (6)	0.0044 (6)	0.0083 (6)
C6	0.0152 (7)	0.0189 (7)	0.0235 (8)	0.0028 (6)	0.0035 (6)	0.0052 (6)
C7	0.0259 (9)	0.0250 (8)	0.0222 (8)	0.0072 (7)	0.0059 (7)	0.0012 (7)
C8	0.0219 (8)	0.0244 (8)	0.0225 (8)	0.0099 (6)	0.0076 (6)	0.0031 (6)
C9	0.0281 (9)	0.0257 (8)	0.0229 (9)	0.0095 (7)	0.0026 (7)	−0.0010 (7)
C10	0.0382 (10)	0.0307 (9)	0.0219 (9)	0.0178 (8)	0.0051 (7)	0.0043 (7)
C11	0.0317 (9)	0.0237 (8)	0.0330 (9)	0.0140 (7)	0.0148 (8)	0.0109 (7)
C12	0.0235 (9)	0.0245 (8)	0.0382 (10)	0.0046 (7)	0.0004 (7)	0.0051 (7)
C13	0.0283 (9)	0.0292 (9)	0.0287 (9)	0.0090 (7)	−0.0007 (7)	0.0079 (7)
C14	0.0172 (8)	0.0250 (8)	0.0273 (9)	0.0038 (6)	0.0074 (7)	0.0043 (7)
C15	0.0176 (8)	0.0226 (8)	0.0193 (8)	0.0067 (6)	0.0034 (6)	0.0057 (6)

Geometric parameters (Å, °)

F1—C11	1.3651 (18)	C4—H4	0.945 (9)
O1—C14	1.2809 (19)	C5—C6	1.392 (2)
O1—H1O	0.861 (10)	C5—C15	1.488 (2)
O2—C14	1.2341 (19)	C6—H6	0.953 (9)
O3—C15	1.2273 (17)	C7—C8	1.514 (2)
O4—C15	1.3156 (17)	C7—H7A	1.001 (9)
O4—H4O	0.868 (9)	C7—H7B	0.990 (9)
N1—C1	1.3728 (19)	C8—C9	1.390 (2)
N1—C7	1.4460 (19)	C8—C13	1.391 (2)
N1—H1N	0.866 (9)	C9—C10	1.387 (2)
C1—C6	1.399 (2)	C9—H9	0.961 (9)
C1—C2	1.405 (2)	C10—C11	1.371 (2)
C2—C3	1.385 (2)	C10—H10	0.952 (9)
C2—H2	0.952 (9)	C11—C12	1.371 (2)
C3—C4	1.394 (2)	C12—C13	1.382 (2)
C3—C14	1.490 (2)	C12—H12	0.958 (9)
C4—C5	1.384 (2)	C13—H13	0.955 (9)
C14—O1—H1O	111.3 (15)	C8—C7—H7B	108.6 (10)
C15—O4—H4O	108.2 (12)	H7A—C7—H7B	105.5 (14)
C1—N1—C7	123.58 (13)	C9—C8—C13	118.46 (15)
C1—N1—H1N	119.1 (13)	C9—C8—C7	122.41 (14)
C7—N1—H1N	116.0 (13)	C13—C8—C7	119.12 (14)
N1—C1—C6	121.89 (13)	C10—C9—C8	121.07 (15)
N1—C1—C2	120.03 (13)	C10—C9—H9	120.6 (10)
C6—C1—C2	118.07 (14)	C8—C9—H9	118.3 (10)

C3—C2—C1	120.61 (14)	C11—C10—C9	118.13 (15)
C3—C2—H2	119.2 (9)	C11—C10—H10	120.4 (11)
C1—C2—H2	120.2 (9)	C9—C10—H10	121.5 (11)
C2—C3—C4	120.87 (13)	F1—C11—C12	118.15 (15)
C2—C3—C14	120.43 (13)	F1—C11—C10	118.95 (15)
C4—C3—C14	118.69 (13)	C12—C11—C10	122.90 (16)
C5—C4—C3	118.82 (13)	C11—C12—C13	118.20 (15)
C5—C4—H4	119.8 (9)	C11—C12—H12	120.2 (11)
C3—C4—H4	121.4 (9)	C13—C12—H12	121.5 (11)
C4—C5—C6	120.82 (13)	C12—C13—C8	121.23 (16)
C4—C5—C15	120.91 (13)	C12—C13—H13	121.3 (10)
C6—C5—C15	118.26 (13)	C8—C13—H13	117.5 (10)
C5—C6—C1	120.73 (13)	O2—C14—O1	123.59 (14)
C5—C6—H6	118.9 (9)	O2—C14—C3	119.88 (14)
C1—C6—H6	120.3 (9)	O1—C14—C3	116.53 (13)
N1—C7—C8	115.64 (13)	O3—C15—O4	123.33 (13)
N1—C7—H7A	110.0 (9)	O3—C15—C5	122.30 (13)
C8—C7—H7A	107.8 (9)	O4—C15—C5	114.37 (12)
N1—C7—H7B	108.8 (10)		
C7—N1—C1—C6	−16.8 (2)	C7—C8—C9—C10	−179.75 (14)
C7—N1—C1—C2	164.21 (15)	C8—C9—C10—C11	−0.5 (2)
N1—C1—C2—C3	−178.04 (14)	C9—C10—C11—F1	179.82 (14)
C6—C1—C2—C3	2.9 (2)	C9—C10—C11—C12	−0.3 (2)
C1—C2—C3—C4	−0.9 (2)	F1—C11—C12—C13	−179.42 (14)
C1—C2—C3—C14	178.51 (14)	C10—C11—C12—C13	0.7 (3)
C2—C3—C4—C5	−1.1 (2)	C11—C12—C13—C8	−0.3 (3)
C14—C3—C4—C5	179.50 (14)	C9—C8—C13—C12	−0.4 (2)
C3—C4—C5—C6	1.0 (2)	C7—C8—C13—C12	−179.85 (15)
C3—C4—C5—C15	−178.08 (13)	C2—C3—C14—O2	−176.06 (16)
C4—C5—C6—C1	1.1 (2)	C4—C3—C14—O2	3.3 (2)
C15—C5—C6—C1	−179.77 (13)	C2—C3—C14—O1	3.2 (2)
N1—C1—C6—C5	177.92 (14)	C4—C3—C14—O1	−177.37 (14)
C2—C1—C6—C5	−3.1 (2)	C4—C5—C15—O3	173.38 (14)
C1—N1—C7—C8	89.38 (19)	C6—C5—C15—O3	−5.7 (2)
N1—C7—C8—C9	−5.7 (2)	C4—C5—C15—O4	−6.4 (2)
N1—C7—C8—C13	173.68 (14)	C6—C5—C15—O4	174.48 (13)
C13—C8—C9—C10	0.8 (2)		

Hydrogen-bond geometry ($\text{\AA}$, $^\circ$)

Cg1 and Cg2 are the centroids of the C1—C6 and C8—C13 benzene rings, respectively.

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
C9—H9 $\cdots$ N1	0.96 (1)	2.52 (1)	2.890 (2)	103 (1)
O1—H1O $\cdots$ O2 ⁱ	0.86 (1)	1.77 (1)	2.6326 (16)	177 (2)
O4—H4O $\cdots$ O3 ⁱⁱ	0.87 (1)	1.79 (1)	2.6518 (15)	176 (2)
N1—H1N $\cdots$ Cg2 ⁱⁱⁱ	0.87 (1)	2.71 (2)	3.4071 (17)	139 (2)

C12—H12...F1 ^{iv}	0.96 (1)	2.46 (1)	3.2661 (19)	142 (1)
C12—H12...O3 ^v	0.96 (1)	2.65 (2)	3.298 (2)	126 (1)

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x+2, -y+1, -z$; (iii) $-x+1, -y+2, -z+1$; (iv) $-x+2, -y+3, -z+1$; (v) $-x+2, -y+2, -z+1$.