

# 4,4'-Difluoro-2,2'-[imidazolidine-1,3-diylbis(methylene)]diphenol

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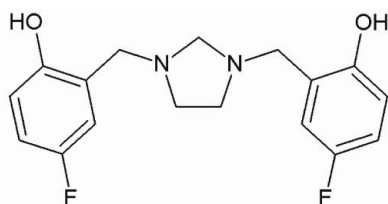
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Key indicators: single-crystal X-ray study;  $T = 120$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.031;  $wR$  factor = 0.108; data-to-parameter ratio = 12.4.

In the title compound,  $\text{C}_{17}\text{H}_{18}\text{F}_2\text{N}_2\text{O}_2$ , the imidazolidine ring system exists in a twist conformation. The mean plane through this ring system forms dihedral angles of  $80.8$  ( $8^\circ$ ) and  $66.2$  ( $13^\circ$ ), with the benzene rings. The dihedral angle between the benzene rings is  $52.0$  ( $14^\circ$ ). Two intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds each generate  $S(6)$  ring motifs. In the crystal, weak  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds form dimers, which are connected by further  $\text{C}-\text{H}\cdots\text{O}$  interactions.

## Related literature

For related structures, see: Rivera *et al.* (2011, 2012). For the preparation of the title compound, see: Rivera *et al.* (1993). For standard bond lengths, see: Allen *et al.* (1987). For ring conformations, see Cremer & Pople (1975). For hydrogen-bond graph-set nomenclature, see: Bernstein *et al.* (1995). For the involvement of organo halides in hydrogen bonds, see: Rathore *et al.* (2011); Steiner (2002); Chopra & Guru Row (2005). For the extinction correction used, see: Becker & Coppens (1974).



## Experimental

### Crystal data

$\text{C}_{17}\text{H}_{18}\text{F}_2\text{N}_2\text{O}_2$   
 $M_r = 320.3$   
 Monoclinic,  $P2_1/n$   
 $a = 9.5952$  (2) Å

$b = 9.7018$  (2) Å  
 $c = 16.2065$  (3) Å  
 $\beta = 99.4807$  ( $17^\circ$ )  
 $V = 1488.07$  (5) Å<sup>3</sup>

$Z = 4$   
 Cu  $K\alpha$  radiation  
 $\mu = 0.94$  mm<sup>-1</sup>

$T = 120$  K  
 $0.35 \times 0.22 \times 0.21$  mm

### Data collection

Agilent Xcalibur (Atlas, Gemini ultra) diffractometer  
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)  
 $T_{\min} = 0.123$ ,  $T_{\max} = 1$

35554 measured reflections  
 2669 independent reflections  
 2452 reflections with  $I > 3\sigma(I)$   
 $R_{\text{int}} = 0.025$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.108$   
 $S = 2.21$   
 2669 reflections  
 215 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.19$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.17$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{N2}$	0.937 (16)	1.756 (16)	2.6413 (12)	156.2 (14)
$\text{O2}-\text{H2}\cdots\text{N1}$	0.903 (16)	1.821 (15)	2.6579 (12)	153.2 (13)
$\text{C11}-\text{H1c11}\cdots\text{O1}^{\text{i}}$	0.96	2.44	3.4001 (13)	174.43
$\text{C17}-\text{H2c17}\cdots\text{O1}^{\text{ii}}$	0.96	2.55	3.4837 (13)	166

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *JANA2006* (Petříček *et al.*, 2006); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *JANA2006*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5264).

## References

- Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.  
 Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.  
 Becker, P. J. & Coppens, P. (1974). *Acta Cryst. A* **30**, 129–147.  
 Bernstein, J., Davis, R. E., Shimon, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.  
 Brandenburg, K. & Putz, H. (2005). *DIAMOND*. Crystal Impact, Bonn, Germany.  
 Chopra, D. & Guru Row, T. N. (2005). *J. Mol. Struct.* **733**, 133–141.  
 Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.  
 Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.  
 Petříček, V., Dusek, M. & Palatinus, L. (2006). *JANA2006*. Institute of Physics, Praha, Czech Republic.  
 Rathore, R. S., Karthikeyan, N. S., Alekhya, Y., Sathiyarayanan, K. & Aravindan, P. G. (2011). *J. Chem. Sci.* **123**, 403–409.  
 Rivera, A., Gallo, G. I., Gayón, M. E. & Joseph-Nathan, P. (1993). *Synth. Commun.* **23**, 2921–2929.

Rivera, A., Nerio, L. S., Ríos-Motta, J., Fejfarová, K. & Dušek, M. (2012). *Acta Cryst.* **E68**, o170–o171.

Rivera, A., Sadat-Bernal, J., Ríos-Motta, J., Pojarová, M. & Dušek, M. (2011). *Acta Cryst.* **E67**, o2581.  
Steiner, T. (2002). *Angew. Chem. Int. Ed.* **41**, 48–76.

## supporting information

*Acta Cryst.* (2012). E68, o3043–o3044 [https://doi.org/10.1107/S1600536812040329]

**4,4'-Difluoro-2,2'-[imidazolidine-1,3-diylbis(methylene)]diphenol**

**Augusto Rivera, Luz Stella Nerio, Jaime Ríos-Motta, Monika Kučeráková and Michal Dušek**

**S1. Comment**

Among the various types of intermolecular interactions, the hydrogen bond is, without doubt, the most important one. Organic halide compounds have attracted much attention due to the role of weak intermolecular C—H $\cdots$ X interactions in supramolecular assembly (Rathore *et al.* 2011, Steiner 2002). In recent literature, the importance of interactions involving fluorine as possible tools in crystal engineering has been explored in greater detail (Chopra & Guru Row, 2005). With the purpose to understand its effects in Mannich bases, we turn our attention to title compound (**I**) because fluorine is also able to form non-classical intermolecular C—H $\cdots$ F hydrogen bonds. In this study, we describe the crystal structure of the title compound, 4,4'-difluoro-2,2'-[imidazolidine-1,3-diylbis(methylene)]diphenol.

The molecular structure and atom-numbering scheme for (**I**) are shown in Fig. 1. The bond lengths (Allen *et al.*, 1987) and angles of (**I**) are within normal ranges and are comparable to those related structures (Rivera *et al.*, 2011, 2012). As observed in related structures (Rivera *et al.*, 2011, 2012). The imidazoline ring adopts a twist conformation,  $Q_2 = 0.4008$  (13) Å and  $\varphi_2 = 51.81$  (18)° (Cremer & Pople, 1975), with a twist about the N2—C14 bond. In order to reduce steric congestion, the benzene rings have different orientations with respect to the central imidazolidine ring. Thus, one *p*-fluoro-substituted benzene ring (C1/C2/C5/C10/C6/C17) is approximately orthogonal to the mean plane of the imidazolidine ring defined by N1, C13 and C9, making a dihedral angle of 80.82 (79)°, whereas the other ring (C3/C4/C7/C13/C16/C12) forms a dihedral angle of 66.18 (130)°. The dihedral angle between the benzene rings is 52.04 (136)°. There are two intramolecular hydrogen bonds between the phenolic hydroxyl groups and the nitrogen atoms with graph-set motif S(6) (Bernstein *et al.*, 1995).

The results demonstrate, that not only the packing in (**I**) is governed by weak C—H $\cdots$ O hydrogen bonds (Table 1), resulting in a hydrogen bonded dimer, which is connected by further C—H $\cdots$ O interactions, but also that fluorine does not participate in any intermolecular interactions. Similarly, in *ortho*-F and *ortho*-Cl substituted analogs (Rivera *et al.*, 2012, 2011), the halogen fails to participate in any non-bonded interaction.

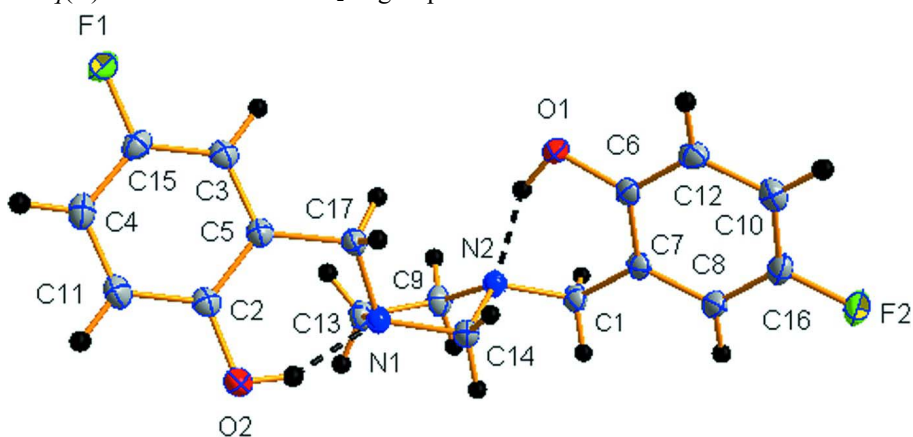
**S2. Experimental**

For the originally reported synthesis of the title compound, see: Rivera *et al.* (1993). Crystals suitable for X-ray diffraction were obtained from chloroform with a few drops of MeOH upon slow evaporation of the solvents over 3 days at room temperature.

**S3. Refinement**

All hydrogen atoms were discernible in difference Fourier maps and could be refined to reasonable geometry. According to common practice H atoms bonded C atoms were kept in ideal positions with C—H distance 0.96 Å during the refinement. The hydroxyl H atoms were found in difference Fourier maps and their coordinates were refined freely. All H atoms were refined with displacement coefficients  $U_{iso}(H)$  set to 1.5 $U_{eq}(C, O)$  for methyl and hydroxyl

groups and to  $1.2U_{eq}(C)$  for the CH— and CH<sub>2</sub>— groups.



**Figure 1**

A perspective view of the title compound, 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. Intramolecular hydrogen bonds are drawn as dashed lines.

#### 4,4'-Difluoro-2,2'-[imidazolidine-1,3-diylbis(methylene)]diphenol

##### Crystal data

C<sub>17</sub>H<sub>18</sub>F<sub>2</sub>N<sub>2</sub>O<sub>2</sub>

$M_r = 320.3$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yabc

$a = 9.5952(2) \text{ \AA}$

$b = 9.7018(2) \text{ \AA}$

$c = 16.2065(3) \text{ \AA}$

$\beta = 99.4807(17)^\circ$

$V = 1488.07(5) \text{ \AA}^3$

$Z = 4$

$F(000) = 672$

$D_x = 1.429 \text{ Mg m}^{-3}$

Cu  $K\alpha$  radiation,  $\lambda = 1.5418 \text{ \AA}$

Cell parameters from 21321 reflections

$\theta = 4.6\text{--}67.0^\circ$

$\mu = 0.94 \text{ mm}^{-1}$

$T = 120 \text{ K}$

Polygon shape, white

$0.35 \times 0.22 \times 0.21 \text{ mm}$

##### Data collection

Agilent Xcalibur (Atlas, Gemini ultra)  
diffractometer

Radiation source: Enhance Ultra (Cu) X-ray  
Source

Mirror monochromator

Detector resolution:  $10.3784 \text{ pixels mm}^{-1}$

$\omega$  scans

Absorption correction: multi-scan  
(*CrysAlis PRO*; Agilent, 2010)

$T_{\min} = 0.123$ ,  $T_{\max} = 1$

35554 measured reflections

2669 independent reflections

2452 reflections with  $I > 3\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 67.1^\circ$ ,  $\theta_{\min} = 5.0^\circ$

$h = -11 \rightarrow 11$

$k = -11 \rightarrow 11$

$l = -19 \rightarrow 19$

##### Refinement

Refinement on  $F^2$

$R[F > 3\sigma(F)] = 0.031$

$wR(F) = 0.108$

$S = 2.21$

2669 reflections

215 parameters

0 restraints

66 constraints

H atoms treated by a mixture of independent  
and constrained refinement

Weighting scheme based on measured s.u.'s  $w =$

$1/(\sigma^2(I) + 0.0016I^2)$

$(\Delta/\sigma)_{\max} = 0.009$

$\Delta\rho_{\max} = 0.19 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.17 \text{ e \AA}^{-3}$

Extinction correction: B-C type 1 Gaussian  
isotropic (Becker & Coppens, 1974)

Extinction coefficient: 900 (400)

*Special details*

**Experimental.** CrysAlisPro, Agilent, 2010

Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**Refinement.** The refinement was carried out against all reflections. The conventional  $R$ -factor is always based on  $F$ . The goodness of fit as well as the weighted  $R$ -factor are based on  $F$  and  $F^2$  for refinement carried out on  $F$  and  $F^2$ , respectively. The threshold expression is used only for calculating  $R$ -factors *etc.* and it is not relevant to the choice of reflections for refinement.

The program used for refinement, Jana2006, uses the weighting scheme based on the experimental expectations, see `_refine_ls_weighting_details`, that does not force  $S$  to be one. Therefore the values of  $S$  are usually larger than the ones from the *SHELX* program.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.58488 (7)	0.98624 (8)	0.11639 (4)	0.0290 (2)
F2	0.02275 (8)	0.97367 (8)	0.76918 (5)	0.0339 (3)
O1	0.37960 (8)	0.95183 (9)	0.53830 (5)	0.0225 (3)
O2	0.14871 (8)	1.28848 (8)	0.20259 (5)	0.0238 (3)
N1	0.25088 (9)	1.23815 (10)	0.36231 (6)	0.0205 (3)
N2	0.32537 (9)	1.21463 (10)	0.50457 (5)	0.0193 (3)
C1	0.30030 (12)	1.22156 (12)	0.59151 (7)	0.0211 (3)
C2	0.25940 (11)	1.21368 (11)	0.18359 (7)	0.0203 (3)
C3	0.45165 (11)	1.05403 (12)	0.21953 (7)	0.0210 (3)
C4	0.39919 (12)	1.14642 (12)	0.07918 (7)	0.0245 (3)
C5	0.33984 (11)	1.12752 (12)	0.24310 (6)	0.0195 (3)
C6	0.28663 (11)	0.96039 (12)	0.59366 (7)	0.0196 (3)
C7	0.24230 (11)	1.08848 (12)	0.62013 (6)	0.0189 (3)
C8	0.15072 (11)	1.09088 (12)	0.67872 (7)	0.0217 (3)
C9	0.40565 (12)	1.33344 (13)	0.48144 (7)	0.0248 (3)
C10	0.14906 (12)	0.84193 (13)	0.68378 (7)	0.0239 (3)
C11	0.29049 (12)	1.22389 (12)	0.10290 (7)	0.0236 (3)
C12	0.23894 (11)	0.83887 (12)	0.62461 (7)	0.0222 (3)
C13	0.36823 (12)	1.33886 (12)	0.38570 (7)	0.0240 (4)
C14	0.19724 (11)	1.21598 (12)	0.44037 (6)	0.0206 (3)
C15	0.47692 (11)	1.06297 (12)	0.13855 (7)	0.0223 (3)
C16	0.10847 (12)	0.96840 (13)	0.70989 (7)	0.0241 (4)
C17	0.30169 (11)	1.10785 (12)	0.32918 (7)	0.0211 (3)
H1c1	0.235801	1.295343	0.597024	0.0253*
H2c1	0.386945	1.24408	0.627648	0.0253*
H1c3	0.510721	0.997491	0.25954	0.0251*
H1c4	0.419502	1.150888	0.023184	0.0294*
H1c8	0.11748	1.177084	0.697131	0.026*
H1c9	0.504952	1.316125	0.497307	0.0297*
H2c9	0.372858	1.415883	0.504826	0.0297*
H1c10	0.116351	0.758191	0.705713	0.0286*
H1c11	0.236448	1.284933	0.063317	0.0283*

H1c12	0.26825	0.751886	0.605019	0.0266*
H1c13	0.335867	1.429715	0.368634	0.0288*
H2c13	0.448556	1.310747	0.361506	0.0288*
H1c14	0.151711	1.127692	0.438843	0.0247*
H2c14	0.138427	1.292231	0.450322	0.0247*
H1c17	0.229709	1.038565	0.326799	0.0253*
H2c17	0.382737	1.074935	0.36675	0.0253*
H2	0.1570 (14)	1.2826 (15)	0.2588 (10)	0.0286*
H1	0.3808 (15)	1.0424 (16)	0.5183 (9)	0.027*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
F1	0.0325 (4)	0.0281 (4)	0.0293 (4)	0.0037 (3)	0.0133 (3)	-0.0034 (3)
F2	0.0408 (4)	0.0331 (5)	0.0338 (4)	0.0006 (3)	0.0235 (3)	0.0031 (3)
O1	0.0263 (4)	0.0211 (5)	0.0221 (4)	0.0031 (3)	0.0096 (3)	-0.0006 (3)
O2	0.0268 (4)	0.0238 (5)	0.0209 (4)	0.0045 (3)	0.0038 (3)	0.0029 (3)
N1	0.0247 (5)	0.0200 (5)	0.0177 (4)	0.0002 (4)	0.0061 (4)	0.0010 (4)
N2	0.0211 (4)	0.0196 (5)	0.0177 (5)	-0.0005 (4)	0.0045 (3)	0.0005 (3)
C1	0.0263 (5)	0.0200 (6)	0.0173 (5)	-0.0004 (4)	0.0045 (4)	-0.0016 (4)
C2	0.0231 (5)	0.0168 (6)	0.0207 (5)	-0.0026 (4)	0.0027 (4)	-0.0006 (4)
C3	0.0240 (5)	0.0170 (6)	0.0214 (6)	-0.0024 (4)	0.0025 (4)	-0.0008 (4)
C4	0.0313 (6)	0.0247 (6)	0.0183 (5)	-0.0058 (5)	0.0067 (4)	-0.0015 (4)
C5	0.0234 (5)	0.0172 (6)	0.0175 (5)	-0.0027 (4)	0.0028 (4)	-0.0008 (4)
C6	0.0191 (5)	0.0235 (6)	0.0155 (5)	0.0010 (4)	0.0011 (4)	-0.0003 (4)
C7	0.0210 (5)	0.0207 (6)	0.0143 (5)	0.0003 (4)	0.0011 (4)	-0.0007 (4)
C8	0.0250 (5)	0.0221 (6)	0.0183 (5)	0.0029 (5)	0.0046 (4)	-0.0010 (4)
C9	0.0281 (6)	0.0228 (6)	0.0242 (6)	-0.0056 (5)	0.0063 (4)	0.0009 (4)
C10	0.0266 (6)	0.0227 (6)	0.0222 (6)	-0.0022 (5)	0.0038 (4)	0.0035 (4)
C11	0.0292 (6)	0.0215 (6)	0.0193 (5)	-0.0027 (5)	0.0015 (4)	0.0028 (4)
C12	0.0261 (6)	0.0199 (6)	0.0201 (5)	0.0020 (4)	0.0022 (4)	-0.0014 (4)
C13	0.0290 (6)	0.0206 (6)	0.0236 (6)	-0.0023 (5)	0.0081 (4)	0.0017 (4)
C14	0.0212 (5)	0.0221 (6)	0.0189 (5)	0.0012 (4)	0.0044 (4)	0.0013 (4)
C15	0.0248 (5)	0.0190 (6)	0.0244 (6)	-0.0028 (4)	0.0075 (4)	-0.0042 (4)
C16	0.0245 (5)	0.0295 (7)	0.0199 (5)	-0.0006 (5)	0.0081 (4)	0.0005 (5)
C17	0.0261 (5)	0.0198 (6)	0.0177 (5)	0.0020 (4)	0.0047 (4)	0.0025 (4)

*Geometric parameters (Å, °)*

F1—C15	1.3706 (14)	C4—H1c4	0.96
F2—C16	1.3648 (15)	C5—C17	1.5116 (16)
O1—C6	1.3680 (14)	C6—C7	1.4034 (16)
O1—H1	0.937 (16)	C6—C12	1.3879 (16)
O2—C2	1.3628 (14)	C7—C8	1.3962 (16)
O2—H2	0.903 (16)	C8—C16	1.3780 (17)
N1—C13	1.4919 (14)	C8—H1c8	0.96
N1—C14	1.4581 (15)	C9—C13	1.5348 (15)
N1—C17	1.4867 (15)	C9—H1c9	0.96

N2—C1	1.4694 (14)	C9—H2c9	0.96
N2—C9	1.4689 (15)	C10—C12	1.3916 (17)
N2—C14	1.4741 (13)	C10—C16	1.3750 (17)
C1—C7	1.5089 (16)	C10—H1c10	0.96
C1—H1c1	0.96	C11—H1c11	0.96
C1—H2c1	0.96	C12—H1c12	0.96
C2—C5	1.4070 (14)	C13—H1c13	0.96
C2—C11	1.3918 (16)	C13—H2c13	0.96
C3—C5	1.3928 (16)	C14—H1c14	0.96
C3—C15	1.3761 (16)	C14—H2c14	0.96
C3—H1c3	0.96	C17—H1c17	0.96
C4—C11	1.3902 (17)	C17—H2c17	0.96
C4—C15	1.3789 (15)		
C6—O1—H1	102.5 (10)	N2—C9—H2c9	109.47
C2—O2—H2	104.6 (9)	C13—C9—H1c9	109.47
C13—N1—C14	103.64 (8)	C13—C9—H2c9	109.47
C13—N1—C17	111.71 (9)	H1c9—C9—H2c9	114.55
C14—N1—C17	111.82 (9)	C12—C10—C16	118.04 (11)
C1—N2—C9	112.60 (8)	C12—C10—H1c10	120.98
C1—N2—C14	115.28 (9)	C16—C10—H1c10	120.98
C9—N2—C14	102.96 (8)	C2—C11—C4	120.53 (10)
N2—C1—C7	112.49 (9)	C2—C11—H1c11	119.73
N2—C1—H1c1	109.47	C4—C11—H1c11	119.73
N2—C1—H2c1	109.47	C6—C12—C10	120.64 (11)
C7—C1—H1c1	109.47	C6—C12—H1c12	119.68
C7—C1—H2c1	109.47	C10—C12—H1c12	119.68
H1c1—C1—H2c1	106.28	N1—C13—C9	105.99 (9)
O2—C2—C5	121.43 (10)	N1—C13—H1c13	109.47
O2—C2—C11	118.03 (9)	N1—C13—H2c13	109.47
C5—C2—C11	120.53 (10)	C9—C13—H1c13	109.47
C5—C3—C15	119.60 (10)	C9—C13—H2c13	109.47
C5—C3—H1c3	120.2	H1c13—C13—H2c13	112.74
C15—C3—H1c3	120.2	N1—C14—N2	103.95 (8)
C11—C4—C15	117.95 (11)	N1—C14—H1c14	109.47
C11—C4—H1c4	121.03	N1—C14—H2c14	109.47
C15—C4—H1c4	121.03	N2—C14—H1c14	109.47
C2—C5—C3	118.46 (10)	N2—C14—H2c14	109.47
C2—C5—C17	121.24 (10)	H1c14—C14—H2c14	114.48
C3—C5—C17	120.20 (9)	F1—C15—C3	118.37 (9)
O1—C6—C7	121.16 (10)	F1—C15—C4	118.77 (10)
O1—C6—C12	118.35 (10)	C3—C15—C4	122.85 (11)
C7—C6—C12	120.48 (10)	F2—C16—C8	118.27 (11)
C1—C7—C6	121.21 (10)	F2—C16—C10	118.96 (11)
C1—C7—C8	120.01 (10)	C8—C16—C10	122.77 (11)
C6—C7—C8	118.62 (10)	N1—C17—C5	111.70 (9)
C7—C8—C16	119.41 (11)	N1—C17—H1c17	109.47
C7—C8—H1c8	120.29	N1—C17—H2c17	109.47

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C16—C8—H1c8	120.29	C5—C17—H1c17	109.47
N2—C9—C13	103.87 (9)	C5—C17—H2c17	109.47
N2—C9—H1c9	109.47	H1c17—C17—H2c17	107.14

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*Hydrogen-bond geometry (Å, °)*

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<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O1—H1...N2	0.937 (16)	1.756 (16)	2.6413 (12)	156.2 (14)
O2—H2...N1	0.903 (16)	1.821 (15)	2.6579 (12)	153.2 (13)
C11—H1c11...O1 <sup>i</sup>	0.96	2.44	3.4001 (13)	174.43
C17—H2c17...O1 <sup>ii</sup>	0.96	2.55	3.4837 (13)	166

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