

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

N,N'-Bis(4-fluorophenyl)urea

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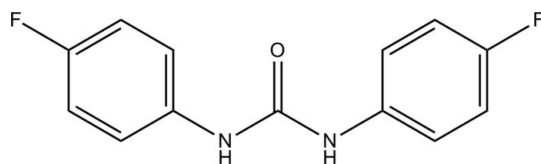
Received 28 April 2010; accepted 5 May 2010

 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.048; wR factor = 0.159; data-to-parameter ratio = 23.3.

The asymmetric unit of the title compound, $\text{C}_{13}\text{H}_{10}\text{F}_2\text{N}_2\text{O}$, contains one and a half *N,N'*-bis(4-fluorophenyl)urea molecules. One of the molecules has crystallographic twofold rotation symmetry. The benzene rings are twisted from each other by dihedral angles of 29.69 (6°) for the molecule in a general position and 89.83 (6°) for the symmetry-generated molecule. In the crystal structure, a pair of intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds link symmetry-related molecules into chains along the b axis, forming $R_2^1(6)$ ring motifs.

Related literature

For background to and the biological activity of bis-aryleureas, see: Khire *et al.* (2004); McDonnell *et al.* (2008); Francisco *et al.* (2004); Bigi *et al.* (1998). For the synthetic method, see: Sarveswari & Raja (2006). For a related structure, see: Jainhuknan *et al.* (1997). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$\text{C}_{13}\text{H}_{10}\text{F}_2\text{N}_2\text{O}$	$c = 10.7098$ (6) Å
$M_r = 248.23$	$\beta = 95.969$ (2°)
Monoclinic, $C2/c$	$V = 3291.4$ (3) Å ³
$a = 67.541$ (4) Å	$Z = 12$
$b = 4.5750$ (3) Å	Mo $K\alpha$ radiation

[‡] Thomson Reuters ResearcherID: C-7581-2009.

[§] Thomson Reuters ResearcherID: A-3561-2009.

 $\mu = 0.12$ mm⁻¹
 $T = 100$ K

 $0.59 \times 0.12 \times 0.09$ mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer	21915 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2009)	5986 independent reflections
$T_{\min} = 0.932$, $T_{\max} = 0.990$	4304 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.159$	$\Delta\rho_{\text{max}} = 0.69$ e Å ⁻³
$S = 1.05$	$\Delta\rho_{\text{min}} = -0.51$ e Å ⁻³
5986 reflections	
257 parameters	

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1A}-\text{H1NA}\cdots\text{O1A}^i$	0.83 (2)	2.08 (2)	2.8331 (13)	151.7 (18)
$\text{N1B}-\text{H1NB}\cdots\text{O1B}^i$	0.89 (3)	2.02 (3)	2.8392 (18)	153.3 (19)
$\text{N2A}-\text{H2NA}\cdots\text{O1A}^i$	0.855 (18)	2.080 (17)	2.8547 (16)	150.5 (13)

 Symmetry code: (i) $x, y + 1, z$.

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

HKF and WSL thank Universiti Sains Malaysia (USM) for the Research University Golden Goose Grant (1001/PFIZIK/811012). WSL thanks the Malaysian Government and USM for the award of Research Fellowship. VV is grateful to the DST-India for funding through the Young Scientist Scheme (Fast Track Proposal).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5040).

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supporting information

Acta Cryst. (2010). E66, o1319 [https://doi.org/10.1107/S1600536810016399]

***N,N'*-Bis(4-fluorophenyl)urea**

Wan-Sin Loh, Hoong-Kun Fun, S. Sarveswari, V. Vijayakumar and R. Venkat Ragavan

S1. Comment

The synthesis of bis-aryureas has received considerable attention due to their wide range of biological applications. They act as potential Raf kinase inhibitors (Khire *et al.*, 2004) and antagonists of human vanilloid receptor 1 (VR 1) (McDonnell *et al.*, 2008). Phenyl thiazolylurea derivatives have been reported as inhibitors of Murine receptor A and Murine receptor B (Francisco *et al.*, 2004). Some substituted ureas are used as antidiabetic and tranquilizing drugs, antioxidants in gasoline, corrosion inhibitor and herbicides (Bigi *et al.*, 1998).

The asymmetric unit of the title compound (Fig. 1), comprises of one and a half *N,N'*-bis-(4-fluorophenyl)urea molecules. The half molecule has a twofold rotation symmetry, generated by symmetry code $-x, y, -z+3/2$. In the molecule with suffix A, both benzene rings (C1A–C6A and C8A–C13A) are twisted from each other with a dihedral angle of 29.69 (6)° whereas in molecule with suffix B, the dihedral angle between the benzene rings (C1B–C6B and C1BA–C6BA) is 89.83 (6)°. The structure is comparable to the related structure (Jai-nhuknan *et al.*, 1997).

In the crystal packing (Fig. 2), intermolecular N1A—H1NA···O1A and N2A—H2NA···O1A hydrogen bonds (Table 1) link the adjacent molecules into chains along the *b* axis, forming $R_2^1(6)$ ring motifs (Bernstein *et al.*, 1995).

S2. Experimental

The compound *N,N'*-bis-(4-fluorophenyl)urea was synthesized using the method available in the literature (Sarveswari & Raja, 2006) and the obtained crude product was recrystallized from absolute ethanol. *M.P.*: 519 K. Yield: 56%.

S3. Refinement

H1NA, H1NB and H2NA were located from a difference Fourier map and refined freely [N–H = 0.83 (2) to 0.88 (3) Å]. The remaining H atoms were positioned geometrically [C–H = 0.93 Å] and were refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$. In the final difference Fourier map, the highest peak is 0.20 Å from atom O1B and the deepest hole is 0.45 Å from atom C7B.

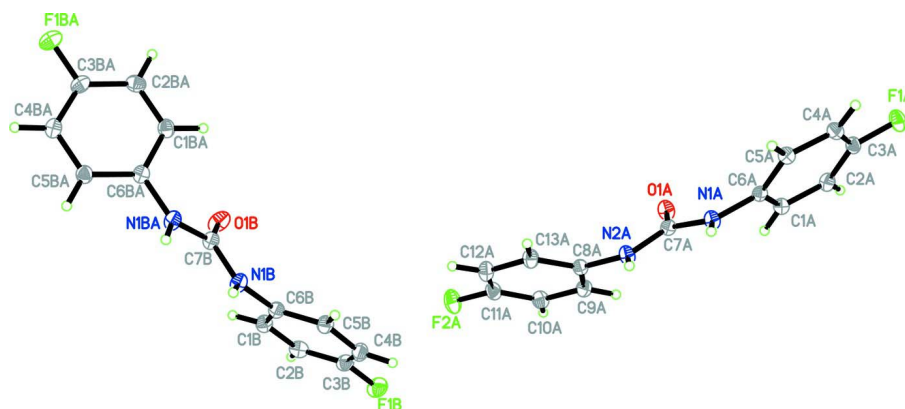


Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme. Atoms with suffix BA [C1BA–C6BA/N1BA/F1BA] are generated by symmetry code $-x, y, -z+3/2$.

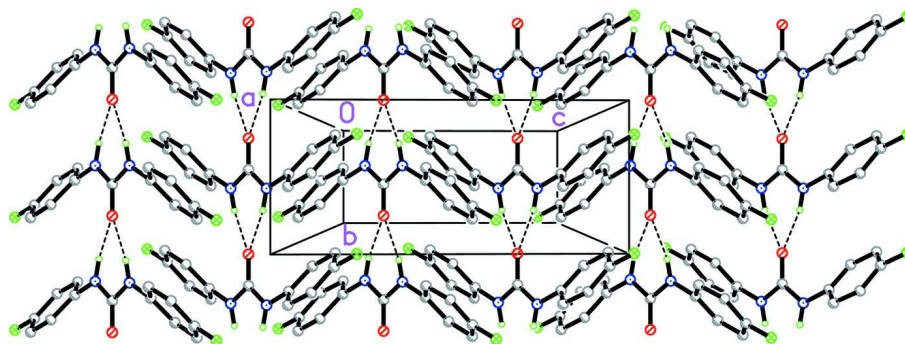


Figure 2

The crystal packing of the title compound, viewed approximately along the a axis, showing $R_2^1(6)$ ring motifs. H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

N,N'-Bis(4-fluorophenyl)urea

Crystal data

$C_{13}H_{10}F_2N_2O$

$M_r = 248.23$

Monoclinic, $C2/c$

Hall symbol: $-C 2yc$

$a = 67.541(4) \text{ \AA}$

$b = 4.5750(3) \text{ \AA}$

$c = 10.7098(6) \text{ \AA}$

$\beta = 95.969(2)^\circ$

$V = 3291.4(3) \text{ \AA}^3$

$Z = 12$

$F(000) = 1536$

$D_x = 1.503 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3635 reflections

$\theta = 2.4\text{--}32.1^\circ$

$\mu = 0.12 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Block, brown

$0.59 \times 0.12 \times 0.09 \text{ mm}$

Data collection

Bruker APEXII DUO CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2009)

$T_{\min} = 0.932$, $T_{\max} = 0.990$

21915 measured reflections

5986 independent reflections

4304 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.050$
 $\theta_{\text{max}} = 32.7^\circ$, $\theta_{\text{min}} = 1.8^\circ$
 $h = -102 \rightarrow 102$

$k = -6 \rightarrow 6$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.159$
 $S = 1.05$
 5986 reflections
 257 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0899P)^2 + 0.1948P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.69 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.51 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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 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(gt) 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.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
F1A	0.244179 (12)	0.5229 (2)	0.33663 (8)	0.02522 (19)
O1A	0.167883 (13)	0.5447 (2)	0.62122 (9)	0.0198 (2)
N1A	0.180685 (15)	0.9777 (2)	0.55991 (10)	0.0162 (2)
N2A	0.153498 (15)	0.9743 (3)	0.67129 (11)	0.0175 (2)
C1A	0.209007 (17)	0.6417 (3)	0.56407 (11)	0.0163 (2)
H1AA	0.2064	0.5746	0.6426	0.020*
C2A	0.225076 (17)	0.5295 (3)	0.50863 (12)	0.0180 (2)
H2AA	0.2332	0.3860	0.5486	0.022*
C3A	0.228714 (17)	0.6362 (3)	0.39263 (12)	0.0178 (2)
C4A	0.217243 (18)	0.8517 (3)	0.33077 (11)	0.0184 (2)
H4AA	0.2203	0.9236	0.2539	0.022*
C5A	0.200924 (18)	0.9591 (3)	0.38612 (11)	0.0172 (2)
H5AA	0.1928	1.1008	0.3451	0.021*
C6A	0.196784 (16)	0.8543 (3)	0.50280 (10)	0.0142 (2)
C7A	0.167422 (16)	0.8158 (3)	0.61783 (11)	0.0150 (2)
C8A	0.138631 (16)	0.8455 (3)	0.73842 (11)	0.0154 (2)
C9A	0.143599 (18)	0.6409 (3)	0.83227 (12)	0.0187 (2)
H9AA	0.1568	0.5838	0.8508	0.022*
C10A	0.128905 (18)	0.5208 (3)	0.89873 (12)	0.0207 (3)

H10A	0.1320	0.3818	0.9610	0.025*
C11A	0.109514 (19)	0.6143 (3)	0.86946 (12)	0.0209 (3)
C12A	0.104185 (18)	0.8202 (3)	0.77910 (12)	0.0219 (3)
H12A	0.0910	0.8809	0.7630	0.026*
C13A	0.118945 (18)	0.9362 (3)	0.71211 (12)	0.0193 (2)
H13A	0.1157	1.0745	0.6497	0.023*
F2A	0.095139 (12)	0.4948 (2)	0.93363 (9)	0.0309 (2)
F1B	0.072613 (12)	0.6424 (2)	1.16351 (8)	0.0289 (2)
O1B	0.0000	0.6661 (3)	0.7500	0.0262 (3)
N1B	0.013863 (16)	1.0982 (3)	0.82126 (11)	0.0193 (2)
C1B	0.024299 (18)	0.7613 (3)	0.99248 (12)	0.0200 (2)
H1BA	0.0112	0.6961	0.9919	0.024*
C2B	0.03907 (2)	0.6455 (3)	1.07851 (12)	0.0213 (3)
H2BA	0.0362	0.4998	1.1343	0.026*
C3B	0.058161 (18)	0.7529 (3)	1.07883 (12)	0.0210 (3)
C4B	0.063141 (18)	0.9679 (3)	0.99790 (12)	0.0212 (3)
H4BA	0.0761	1.0385	1.0018	0.025*
C5B	0.048369 (18)	1.0776 (3)	0.91008 (12)	0.0194 (2)
H5BA	0.0515	1.2200	0.8533	0.023*
C6B	0.028914 (17)	0.9741 (3)	0.90722 (12)	0.0170 (2)
C7B	0.0000	0.9380 (4)	0.7500	0.0181 (3)
H1NA	0.1792 (3)	1.157 (5)	0.5567 (17)	0.028 (5)*
H1NB	0.0136 (3)	1.289 (6)	0.8078 (19)	0.043 (6)*
H2NA	0.1535 (2)	1.160 (4)	0.6624 (16)	0.022 (4)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1A	0.0210 (3)	0.0251 (5)	0.0312 (4)	0.0051 (3)	0.0105 (3)	-0.0019 (4)
O1A	0.0215 (4)	0.0090 (4)	0.0302 (5)	-0.0003 (3)	0.0084 (3)	-0.0003 (4)
N1A	0.0180 (4)	0.0082 (5)	0.0231 (5)	0.0010 (4)	0.0059 (4)	0.0014 (4)
N2A	0.0184 (4)	0.0094 (5)	0.0258 (5)	0.0014 (4)	0.0076 (4)	0.0010 (4)
C1A	0.0170 (5)	0.0144 (6)	0.0175 (5)	0.0004 (4)	0.0018 (4)	0.0011 (4)
C2A	0.0159 (5)	0.0147 (6)	0.0232 (6)	0.0025 (4)	0.0015 (4)	0.0012 (5)
C3A	0.0148 (5)	0.0171 (6)	0.0220 (5)	0.0005 (4)	0.0040 (4)	-0.0041 (5)
C4A	0.0195 (5)	0.0187 (6)	0.0174 (5)	-0.0004 (5)	0.0046 (4)	0.0001 (5)
C5A	0.0183 (5)	0.0151 (6)	0.0181 (5)	0.0007 (5)	0.0021 (4)	0.0006 (4)
C6A	0.0150 (4)	0.0106 (5)	0.0170 (5)	-0.0005 (4)	0.0017 (4)	-0.0015 (4)
C7A	0.0153 (4)	0.0119 (5)	0.0178 (5)	0.0006 (4)	0.0015 (4)	-0.0001 (4)
C8A	0.0157 (4)	0.0114 (5)	0.0195 (5)	-0.0011 (4)	0.0039 (4)	-0.0013 (4)
C9A	0.0178 (5)	0.0176 (6)	0.0205 (5)	-0.0003 (5)	0.0016 (4)	0.0011 (5)
C10A	0.0212 (5)	0.0207 (7)	0.0205 (6)	0.0006 (5)	0.0039 (4)	0.0035 (5)
C11A	0.0201 (5)	0.0200 (6)	0.0239 (6)	-0.0038 (5)	0.0078 (4)	-0.0015 (5)
C12A	0.0161 (5)	0.0215 (7)	0.0286 (6)	0.0010 (5)	0.0044 (4)	0.0005 (5)
C13A	0.0174 (5)	0.0168 (6)	0.0238 (6)	0.0019 (5)	0.0030 (4)	0.0020 (5)
F2A	0.0247 (4)	0.0319 (5)	0.0384 (5)	-0.0037 (4)	0.0150 (3)	0.0060 (4)
F1B	0.0284 (4)	0.0301 (5)	0.0263 (4)	0.0062 (4)	-0.0060 (3)	0.0031 (4)
O1B	0.0302 (7)	0.0107 (6)	0.0351 (7)	0.000	-0.0093 (6)	0.000

N1B	0.0177 (4)	0.0112 (5)	0.0280 (5)	-0.0008 (4)	-0.0017 (4)	0.0004 (4)
C1B	0.0194 (5)	0.0172 (6)	0.0235 (6)	-0.0020 (5)	0.0031 (4)	-0.0001 (5)
C2B	0.0275 (6)	0.0165 (6)	0.0200 (5)	-0.0009 (5)	0.0029 (4)	0.0015 (5)
C3B	0.0216 (5)	0.0203 (6)	0.0201 (5)	0.0039 (5)	-0.0024 (4)	-0.0008 (5)
C4B	0.0168 (5)	0.0223 (7)	0.0244 (6)	-0.0004 (5)	0.0011 (4)	-0.0012 (5)
C5B	0.0184 (5)	0.0180 (6)	0.0218 (5)	-0.0010 (5)	0.0022 (4)	0.0007 (5)
C6B	0.0171 (5)	0.0123 (6)	0.0213 (5)	0.0007 (4)	0.0010 (4)	-0.0016 (4)
C7B	0.0170 (7)	0.0136 (8)	0.0234 (8)	0.000	0.0005 (6)	0.000

Geometric parameters (Å, °)

F1A—C3A	1.3601 (13)	C10A—H10A	0.9300
O1A—C7A	1.2412 (15)	C11A—F2A	1.3611 (14)
N1A—C7A	1.3606 (15)	C11A—C12A	1.371 (2)
N1A—C6A	1.4190 (15)	C12A—C13A	1.3925 (17)
N1A—H1NA	0.83 (2)	C12A—H12A	0.9300
N2A—C7A	1.3602 (15)	C13A—H13A	0.9300
N2A—C8A	1.4223 (15)	F1B—C3B	1.3589 (15)
N2A—H2NA	0.85 (2)	O1B—C7B	1.244 (2)
C1A—C2A	1.3886 (16)	N1B—C7B	1.3593 (15)
C1A—C6A	1.3948 (17)	N1B—C6B	1.4173 (16)
C1A—H1AA	0.9300	N1B—H1NB	0.88 (3)
C2A—C3A	1.3805 (18)	C1B—C2B	1.3902 (18)
C2A—H2AA	0.9300	C1B—C6B	1.3921 (18)
C3A—C4A	1.3799 (18)	C1B—H1BA	0.9300
C4A—C5A	1.3941 (16)	C2B—C3B	1.3798 (19)
C4A—H4AA	0.9300	C2B—H2BA	0.9300
C5A—C6A	1.3937 (16)	C3B—C4B	1.376 (2)
C5A—H5AA	0.9300	C4B—C5B	1.3916 (18)
C8A—C9A	1.3888 (18)	C4B—H4BA	0.9300
C8A—C13A	1.3935 (16)	C5B—C6B	1.3942 (17)
C9A—C10A	1.3929 (17)	C5B—H5BA	0.9300
C9A—H9AA	0.9300	C7B—N1B ⁱ	1.3593 (15)
C10A—C11A	1.3824 (18)		
C7A—N1A—C6A	123.39 (11)	C9A—C10A—H10A	121.0
C7A—N1A—H1NA	118.3 (13)	F2A—C11A—C12A	118.92 (12)
C6A—N1A—H1NA	118.3 (13)	F2A—C11A—C10A	118.03 (12)
C7A—N2A—C8A	123.17 (11)	C12A—C11A—C10A	123.05 (12)
C7A—N2A—H2NA	118.4 (11)	C11A—C12A—C13A	118.42 (12)
C8A—N2A—H2NA	118.4 (11)	C11A—C12A—H12A	120.8
C2A—C1A—C6A	120.49 (11)	C13A—C12A—H12A	120.8
C2A—C1A—H1AA	119.8	C12A—C13A—C8A	120.09 (12)
C6A—C1A—H1AA	119.8	C12A—C13A—H13A	120.0
C3A—C2A—C1A	118.30 (11)	C8A—C13A—H13A	120.0
C3A—C2A—H2AA	120.8	C7B—N1B—C6B	123.66 (12)
C1A—C2A—H2AA	120.8	C7B—N1B—H1NB	116.0 (14)
F1A—C3A—C4A	118.63 (11)	C6B—N1B—H1NB	120.2 (14)

F1A—C3A—C2A	118.60 (11)	C2B—C1B—C6B	120.46 (11)
C4A—C3A—C2A	122.77 (11)	C2B—C1B—H1BA	119.8
C3A—C4A—C5A	118.48 (11)	C6B—C1B—H1BA	119.8
C3A—C4A—H4AA	120.8	C3B—C2B—C1B	118.17 (13)
C5A—C4A—H4AA	120.8	C3B—C2B—H2BA	120.9
C6A—C5A—C4A	120.08 (12)	C1B—C2B—H2BA	120.9
C6A—C5A—H5AA	120.0	F1B—C3B—C4B	118.73 (12)
C4A—C5A—H5AA	120.0	F1B—C3B—C2B	118.40 (13)
C5A—C6A—C1A	119.84 (11)	C4B—C3B—C2B	122.87 (12)
C5A—C6A—N1A	118.94 (11)	C3B—C4B—C5B	118.59 (12)
C1A—C6A—N1A	121.14 (10)	C3B—C4B—H4BA	120.7
O1A—C7A—N2A	122.47 (11)	C5B—C4B—H4BA	120.7
O1A—C7A—N1A	122.79 (11)	C4B—C5B—C6B	120.01 (13)
N2A—C7A—N1A	114.74 (11)	C4B—C5B—H5BA	120.0
C9A—C8A—C13A	120.06 (11)	C6B—C5B—H5BA	120.0
C9A—C8A—N2A	121.00 (10)	C1B—C6B—C5B	119.87 (12)
C13A—C8A—N2A	118.90 (11)	C1B—C6B—N1B	120.79 (11)
C8A—C9A—C10A	120.28 (11)	C5B—C6B—N1B	119.26 (12)
C8A—C9A—H9AA	119.9	O1B—C7B—N1B ⁱ	122.63 (9)
C10A—C9A—H9AA	119.9	O1B—C7B—N1B	122.63 (8)
C11A—C10A—C9A	118.08 (12)	N1B ⁱ —C7B—N1B	114.74 (17)
C11A—C10A—H10A	121.0		

Symmetry code: (i) $-x, y, -z+3/2$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1A—H1NA \cdots O1A ⁱⁱ	0.83 (2)	2.08 (2)	2.8331 (13)	151.7 (18)
N1B—H1NB \cdots O1B ⁱⁱ	0.89 (3)	2.02 (3)	2.8392 (18)	153.3 (19)
N2A—H2NA \cdots O1A ⁱⁱ	0.855 (18)	2.080 (17)	2.8547 (16)	150.5 (13)

Symmetry code: (ii) $x, y+1, z$.