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2,2-Diphenyl-*N*-(2,4,5-trichlorophenyl)-acetamide

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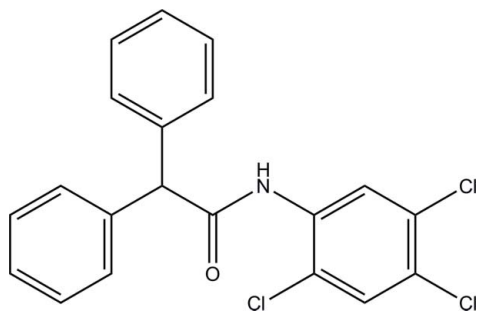
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.047; wR factor = 0.114; data-to-parameter ratio = 23.3.

The asymmetric unit of the title compound, $\text{C}_{20}\text{H}_{14}\text{Cl}_3\text{NO}$, consists of two independent molecules. In one molecule, the chlorinated benzene ring forms dihedral angles of 12.00 (9) and 77.04 (9)° with the phenyl rings. The dihedral angle between the phenyl rings is 80.37 (10)°. The corresponding dihedral angles for the other molecule are 26.34 (10), 62.98 (10) and 88.47 (11)°, respectively. One of the molecules features an intramolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond, which forms an $S(6)$ ring motif. In the crystal, molecules are linked by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds into [100] chains. The chains are further linked by $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds into a three-dimensional network.

Related literature

For general background to and related structures of the title compound, see: Fun *et al.* (2011*a,b*, 2012*a,b*). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



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§ Thomson Reuters ResearcherID: A-5525-2009.

Experimental

Crystal data

$\text{C}_{20}\text{H}_{14}\text{Cl}_3\text{NO}$
 $M_r = 390.67$
 Orthorhombic, $Pbca$
 $a = 18.6630$ (16) Å
 $b = 17.1713$ (15) Å
 $c = 22.5648$ (19) Å
 $V = 7231.3$ (11) Å³
 $Z = 16$
 Mo $K\alpha$ radiation
 $\mu = 0.51$ mm⁻¹
 $T = 100$ K
 $0.38 \times 0.14 \times 0.11$ mm

Data collection

Bruker SMART APEXII DUO CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
 $T_{\min} = 0.830$, $T_{\max} = 0.946$
 45180 measured reflections
 10676 independent reflections
 7536 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.076$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.114$
 $S = 1.02$
 10676 reflections
 459 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.52$ e Å⁻³
 $\Delta\rho_{\min} = -0.49$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1A}-\text{H1NA}\cdots\text{O1B}^i$	0.78 (2)	2.09 (2)	2.8379 (19)	161 (2)
$\text{N1B}-\text{H1NB}\cdots\text{O1A}$	0.84 (2)	1.94 (2)	2.7684 (19)	168 (2)
$\text{C7A}-\text{H7AA}\cdots\text{O1B}^i$	1.00	2.33	3.234 (2)	151
$\text{C1B}-\text{H1BA}\cdots\text{O1B}$	0.95	2.48	3.116 (3)	125
$\text{C3B}-\text{H3BA}\cdots\text{O1B}^{ii}$	0.95	2.42	3.368 (3)	172
$\text{C12B}-\text{H12B}\cdots\text{Cl2B}^{iii}$	0.95	2.82	3.641 (3)	145
$\text{C7B}-\text{H7BA}\cdots\text{O1A}$	1.00	2.46	3.341 (2)	147

Symmetry codes: (i) $x + \frac{1}{2}, y, -z + \frac{1}{2}$; (ii) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$; (iii) $x, -y + \frac{5}{2}, z + \frac{1}{2}$.

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6924).

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supporting information

Acta Cryst. (2012). E68, o2659–o2660 [doi:10.1107/S160053681203440X]

2,2-Diphenyl-*N*-(2,4,5-trichlorophenyl)acetamide

Hoong-Kun Fun, Ching Kheng Quah, Prakash S. Nayak, B. Narayana and B. K. Sarojini

S1. Comment

In continuation of our work on synthesis of amides (Fun *et al.*, 2011*a*, 2011*b*, 2012*a*, 2012*b*), we report herein the crystal structure of the title compound.

The asymmetric unit (Fig. 1) of the title compound consists of two independent molecules (*A* and *B*), with comparable geometries. In molecule *A*, the benzene ring (C15A–C20A) forms dihedral angles of 12.00 (9) and 77.04 (9)° with two phenyl rings (C1A–C6A and C8A–C13A). The dihedral angle between two phenyl rings is 80.37 (10)°. The corresponding dihedral angles for molecule *B* are 26.34 (10), 62.98 (10) and 88.47 (11)°, respectively. Bond lengths and angles are within normal ranges and are comparable to related structures (Fun *et al.*, 2011*a*, 2011*b*, 2012*a*, 2012*b*). The molecular structure is stabilized by intramolecular C1B–H1BA⋯O1B hydrogen bond, forming an S(6) ring motif (Bernstein *et al.*, 1995).

In the crystal structure, Fig. 2, molecules are linked by N1A–H1NA⋯O1B, N1B–H1NB⋯O1A, C7A–H7AA⋯O1B, C3B–H3BA⋯O1B, C12B–H12B⋯C12B and C7B–H7BA⋯O1A hydrogen bonds (Table 1) into a three-dimensional network.

S2. Experimental

Diphenylacetic acid (0.212 g, 1 mmol), 2,4,5-trichloroaniline (0.196 g, 1 mmol) and 1-ethyl-3-(3-dimethylaminopropyl)-carbodiimide hydrochloride (1.0 g, 0.01 mol) were dissolved in dichloromethane (20 ml). The mixture was stirred in the presence of triethylamine at 273 K for about 3 h. The contents were poured into 100 ml of ice-cold aqueous hydrochloric acid with stirring. The concoction was extracted thrice with dichloromethane. The organic layer was washed with saturated NaHCO₃ solution and brine solution, dried and concentrated under reduced pressure to give the title compound (I). Colourless needles were grown from ethanol solution by the slow evaporation method (*m.p.*: 391–393K).

S3. Refinement

N-bound H atoms were located in a difference Fourier map and refined freely [N–H = 0.78 (2) or 0.84 (2) Å]. The remaining H atoms were positioned geometrically and refined using a riding model with C–H = 0.95 or 1.00 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

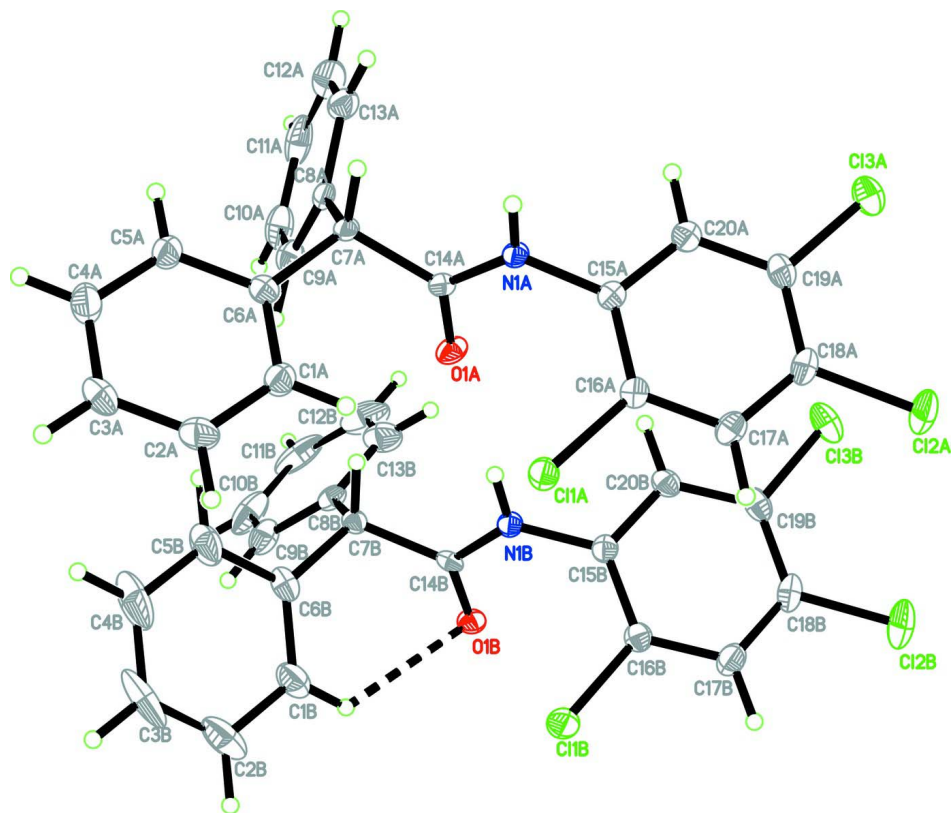


Figure 1

The asymmetric unit of the title compound showing 50% probability displacement ellipsoids for non-H atoms. Intramolecular hydrogen bond is shown as dashed line.

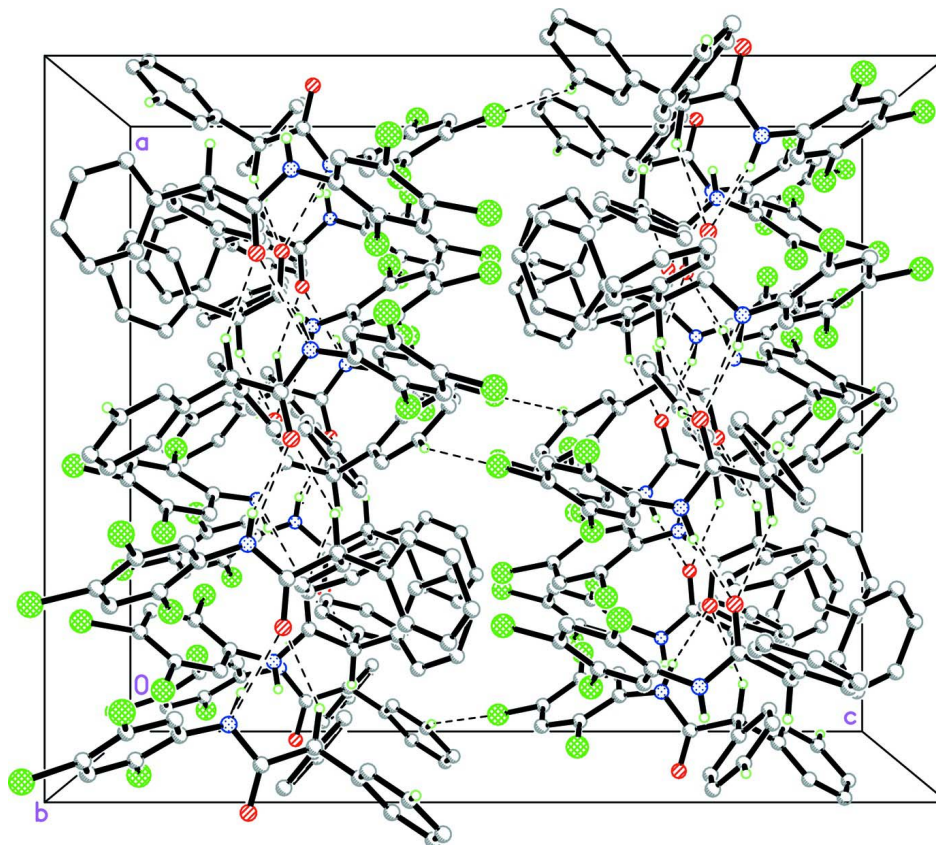


Figure 2

The crystal structure of the title compound, viewed along the *b* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

2,2-Diphenyl-*N*-(2,4,5-trichlorophenyl)acetamide

Crystal data

$C_{20}H_{14}Cl_3NO$

$M_r = 390.67$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 18.6630$ (16) Å

$b = 17.1713$ (15) Å

$c = 22.5648$ (19) Å

$V = 7231.3$ (11) Å³

$Z = 16$

$F(000) = 3200$

$D_x = 1.435$ Mg m⁻³

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

Cell parameters from 6747 reflections

$\theta = 2.4$ – 29.9°

$\mu = 0.51$ mm⁻¹

$T = 100$ K

Needle, colourless

$0.38 \times 0.14 \times 0.11$ mm

Data collection

Bruker SMART APEXII DUO CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

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

$T_{\min} = 0.830$, $T_{\max} = 0.946$

45180 measured reflections

10676 independent reflections

7536 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.076$

$\theta_{\max} = 30.2^\circ$, $\theta_{\min} = 1.8^\circ$

$h = -26 \rightarrow 25$

$k = -15 \rightarrow 24$

$l = -28 \rightarrow 31$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.114$
 $S = 1.02$
 10676 reflections
 459 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
 $w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 2.0216P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.52 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.49 \text{ e } \text{Å}^{-3}$

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 $F^2 > 2\sigma(F^2)$ 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 (Å^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1A	0.25176 (2)	0.93641 (3)	0.13414 (2)	0.01907 (10)
Cl2A	0.27575 (3)	1.19747 (3)	0.00787 (2)	0.02842 (12)
Cl3A	0.36832 (3)	1.27469 (3)	0.11150 (2)	0.02949 (12)
O1A	0.23516 (6)	1.01068 (8)	0.26465 (6)	0.0181 (3)
N1A	0.34664 (8)	1.01920 (9)	0.22602 (7)	0.0137 (3)
C1A	0.28328 (10)	0.83104 (12)	0.27665 (9)	0.0210 (4)
H1AA	0.2713	0.8590	0.2417	0.025*
C2A	0.27020 (11)	0.75132 (13)	0.27947 (9)	0.0246 (4)
H2AA	0.2492	0.7256	0.2465	0.030*
C3A	0.28742 (10)	0.70921 (12)	0.32957 (9)	0.0236 (4)
H3AA	0.2783	0.6548	0.3314	0.028*
C4A	0.31836 (11)	0.74771 (13)	0.37728 (9)	0.0265 (4)
H4AA	0.3308	0.7194	0.4119	0.032*
C5A	0.33122 (11)	0.82721 (12)	0.37473 (8)	0.0217 (4)
H5AA	0.3523	0.8527	0.4077	0.026*
C6A	0.31349 (9)	0.87024 (11)	0.32420 (8)	0.0150 (3)
C7A	0.33187 (9)	0.95686 (10)	0.32258 (7)	0.0131 (3)
H7AA	0.3852	0.9615	0.3198	0.016*
C8A	0.30808 (9)	1.00164 (11)	0.37751 (8)	0.0149 (3)
C9A	0.23862 (10)	0.99421 (12)	0.39993 (8)	0.0208 (4)
H9AA	0.2064	0.9578	0.3828	0.025*
C10A	0.21668 (12)	1.04027 (13)	0.44749 (9)	0.0281 (5)

H10A	0.1692	1.0357	0.4623	0.034*
C11A	0.26365 (14)	1.09258 (14)	0.47326 (9)	0.0345 (6)
H11A	0.2483	1.1241	0.5055	0.041*
C12A	0.33262 (14)	1.09906 (13)	0.45230 (10)	0.0323 (5)
H12A	0.3651	1.1342	0.4706	0.039*
C13A	0.35485 (11)	1.05418 (12)	0.40421 (9)	0.0233 (4)
H13A	0.4023	1.0595	0.3895	0.028*
C14A	0.29980 (9)	0.99760 (10)	0.26836 (7)	0.0129 (3)
C15A	0.32606 (9)	1.06227 (11)	0.17496 (7)	0.0135 (3)
C16A	0.28376 (9)	1.03068 (11)	0.12995 (8)	0.0148 (3)
C17A	0.26736 (10)	1.07342 (12)	0.07947 (8)	0.0185 (4)
H17A	0.2379	1.0514	0.0495	0.022*
C18A	0.29391 (10)	1.14804 (12)	0.07292 (8)	0.0185 (4)
C19A	0.33520 (10)	1.18112 (11)	0.11770 (8)	0.0189 (4)
C20A	0.35102 (9)	1.13825 (11)	0.16837 (8)	0.0171 (4)
H20A	0.3792	1.1611	0.1988	0.020*
C11B	0.03020 (3)	0.94169 (3)	0.09896 (2)	0.02343 (11)
C12B	0.05234 (3)	1.22599 (4)	0.00236 (2)	0.03695 (14)
C13B	0.14530 (3)	1.28165 (3)	0.11307 (2)	0.02957 (12)
O1B	-0.01287 (6)	1.01048 (8)	0.22632 (6)	0.0165 (3)
N1B	0.10563 (8)	1.01476 (9)	0.20494 (7)	0.0149 (3)
C1B	0.00063 (12)	0.83378 (13)	0.25576 (9)	0.0279 (5)
H1BA	-0.0283	0.8675	0.2325	0.034*
C2B	-0.01116 (14)	0.75387 (14)	0.25393 (11)	0.0385 (6)
H2BA	-0.0481	0.7332	0.2296	0.046*
C3B	0.03066 (13)	0.70482 (13)	0.28732 (13)	0.0423 (7)
H3BA	0.0223	0.6503	0.2863	0.051*
C4B	0.08436 (13)	0.73425 (14)	0.32218 (14)	0.0465 (7)
H4BA	0.1135	0.7001	0.3449	0.056*
C5B	0.09604 (11)	0.81390 (13)	0.32417 (11)	0.0333 (5)
H5BA	0.1333	0.8340	0.3485	0.040*
C6B	0.05443 (9)	0.86469 (11)	0.29132 (8)	0.0187 (4)
C7B	0.06907 (9)	0.95122 (10)	0.29632 (8)	0.0144 (3)
H7BA	0.1218	0.9576	0.3024	0.017*
C8B	0.03170 (9)	0.99156 (11)	0.34826 (8)	0.0171 (4)
C9B	-0.01905 (10)	0.95404 (13)	0.38322 (9)	0.0249 (4)
H9BA	-0.0318	0.9016	0.3751	0.030*
C10B	-0.05113 (12)	0.99360 (17)	0.43017 (9)	0.0370 (6)
H10B	-0.0853	0.9676	0.4543	0.044*
C11B	-0.03377 (13)	1.06999 (18)	0.44199 (10)	0.0423 (7)
H11B	-0.0557	1.0965	0.4742	0.051*
C12B	0.01588 (13)	1.10794 (16)	0.40664 (11)	0.0413 (6)
H12B	0.0276	1.1608	0.4142	0.050*
C13B	0.04849 (12)	1.06879 (13)	0.36023 (10)	0.0295 (5)
H13B	0.0827	1.0951	0.3363	0.035*
C14B	0.04969 (9)	0.99439 (10)	0.23948 (8)	0.0133 (3)
C15B	0.09611 (9)	1.06242 (11)	0.15425 (8)	0.0151 (3)
C16B	0.05996 (10)	1.03687 (11)	0.10398 (8)	0.0169 (4)

C17B	0.04756 (10)	1.08745 (12)	0.05716 (8)	0.0220 (4)
H17B	0.0220	1.0700	0.0233	0.026*
C18B	0.07236 (10)	1.16331 (12)	0.05979 (8)	0.0221 (4)
C19B	0.11177 (10)	1.18824 (11)	0.10842 (9)	0.0200 (4)
C20B	0.12309 (9)	1.13779 (11)	0.15547 (8)	0.0178 (4)
H20B	0.1496	1.1550	0.1889	0.021*
H1NA	0.3879 (12)	1.0179 (13)	0.2313 (10)	0.024 (6)*
H1NB	0.1474 (12)	1.0101 (13)	0.2186 (10)	0.022 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11A	0.0270 (2)	0.0140 (2)	0.0162 (2)	-0.00103 (17)	-0.00160 (17)	-0.00142 (16)
C12A	0.0418 (3)	0.0240 (3)	0.0194 (2)	0.0052 (2)	-0.0025 (2)	0.00825 (19)
C13A	0.0362 (3)	0.0173 (2)	0.0349 (3)	-0.0061 (2)	-0.0022 (2)	0.0071 (2)
O1A	0.0105 (6)	0.0288 (8)	0.0151 (6)	0.0016 (5)	-0.0005 (5)	0.0017 (5)
N1A	0.0081 (7)	0.0183 (8)	0.0146 (7)	0.0008 (6)	0.0000 (5)	0.0031 (6)
C1A	0.0255 (9)	0.0192 (10)	0.0183 (9)	-0.0003 (8)	-0.0026 (8)	0.0003 (7)
C2A	0.0264 (10)	0.0216 (11)	0.0257 (10)	-0.0030 (8)	-0.0025 (8)	-0.0063 (8)
C3A	0.0233 (9)	0.0151 (10)	0.0325 (11)	-0.0017 (8)	0.0054 (8)	-0.0011 (8)
C4A	0.0342 (11)	0.0205 (11)	0.0248 (11)	-0.0007 (9)	0.0000 (8)	0.0048 (8)
C5A	0.0281 (10)	0.0199 (10)	0.0172 (9)	-0.0021 (8)	-0.0035 (8)	0.0014 (8)
C6A	0.0116 (7)	0.0163 (9)	0.0169 (9)	0.0007 (7)	0.0025 (6)	-0.0007 (7)
C7A	0.0097 (7)	0.0166 (9)	0.0129 (8)	-0.0008 (6)	-0.0004 (6)	0.0017 (7)
C8A	0.0196 (8)	0.0139 (9)	0.0113 (8)	0.0011 (7)	-0.0020 (6)	0.0023 (6)
C9A	0.0233 (9)	0.0242 (11)	0.0150 (9)	0.0021 (8)	0.0021 (7)	0.0024 (8)
C10A	0.0366 (12)	0.0296 (12)	0.0182 (10)	0.0110 (10)	0.0091 (8)	0.0058 (8)
C11A	0.0682 (17)	0.0205 (12)	0.0149 (10)	0.0140 (11)	0.0021 (10)	0.0006 (8)
C12A	0.0540 (15)	0.0186 (11)	0.0242 (11)	-0.0014 (10)	-0.0103 (10)	-0.0036 (9)
C13A	0.0288 (10)	0.0192 (10)	0.0217 (10)	-0.0007 (8)	-0.0068 (8)	-0.0001 (8)
C14A	0.0118 (7)	0.0141 (9)	0.0126 (8)	-0.0006 (6)	-0.0008 (6)	-0.0012 (6)
C15A	0.0108 (7)	0.0171 (9)	0.0125 (8)	0.0032 (6)	0.0023 (6)	-0.0010 (7)
C16A	0.0156 (8)	0.0136 (9)	0.0152 (8)	0.0030 (7)	0.0021 (6)	-0.0012 (7)
C17A	0.0213 (9)	0.0199 (10)	0.0143 (9)	0.0041 (7)	-0.0002 (7)	-0.0017 (7)
C18A	0.0208 (9)	0.0199 (10)	0.0149 (9)	0.0063 (7)	0.0022 (7)	0.0036 (7)
C19A	0.0196 (9)	0.0147 (9)	0.0224 (9)	0.0006 (7)	0.0035 (7)	0.0025 (7)
C20A	0.0157 (8)	0.0192 (10)	0.0163 (9)	0.0014 (7)	0.0022 (7)	-0.0002 (7)
C11B	0.0310 (2)	0.0175 (2)	0.0218 (2)	-0.00232 (19)	-0.00480 (19)	-0.00196 (18)
C12B	0.0515 (3)	0.0325 (3)	0.0269 (3)	0.0077 (3)	0.0011 (2)	0.0155 (2)
C13B	0.0337 (3)	0.0162 (2)	0.0388 (3)	-0.0046 (2)	0.0087 (2)	0.0030 (2)
O1B	0.0105 (5)	0.0190 (7)	0.0202 (7)	0.0003 (5)	-0.0017 (5)	0.0006 (5)
N1B	0.0090 (7)	0.0190 (8)	0.0166 (8)	-0.0003 (6)	-0.0006 (6)	0.0040 (6)
C1B	0.0356 (11)	0.0189 (11)	0.0294 (11)	-0.0075 (9)	0.0040 (9)	-0.0025 (8)
C2B	0.0474 (14)	0.0222 (12)	0.0457 (14)	-0.0140 (11)	0.0154 (11)	-0.0112 (10)
C3B	0.0407 (13)	0.0121 (11)	0.0743 (19)	-0.0034 (10)	0.0377 (13)	-0.0022 (11)
C4B	0.0315 (12)	0.0209 (13)	0.087 (2)	0.0072 (10)	0.0160 (13)	0.0204 (13)
C5B	0.0228 (10)	0.0209 (11)	0.0562 (15)	0.0019 (9)	-0.0001 (10)	0.0132 (10)
C6B	0.0165 (8)	0.0146 (9)	0.0249 (10)	0.0015 (7)	0.0077 (7)	0.0009 (7)

C7B	0.0106 (7)	0.0141 (9)	0.0184 (9)	-0.0005 (6)	0.0000 (6)	0.0014 (7)
C8B	0.0156 (8)	0.0194 (10)	0.0165 (9)	0.0049 (7)	-0.0047 (7)	-0.0011 (7)
C9B	0.0220 (9)	0.0321 (12)	0.0207 (10)	0.0073 (8)	0.0013 (8)	0.0046 (8)
C10B	0.0299 (11)	0.0636 (19)	0.0175 (10)	0.0184 (11)	0.0025 (9)	0.0057 (11)
C11B	0.0391 (13)	0.068 (2)	0.0196 (11)	0.0304 (13)	-0.0111 (10)	-0.0171 (11)
C12B	0.0428 (14)	0.0407 (15)	0.0404 (14)	0.0151 (12)	-0.0165 (11)	-0.0225 (12)
C13B	0.0303 (11)	0.0264 (12)	0.0319 (12)	-0.0005 (9)	-0.0056 (9)	-0.0088 (9)
C14B	0.0116 (7)	0.0102 (8)	0.0180 (8)	-0.0024 (6)	0.0000 (6)	-0.0023 (6)
C15B	0.0119 (8)	0.0171 (9)	0.0162 (8)	0.0017 (7)	0.0006 (6)	0.0023 (7)
C16B	0.0170 (8)	0.0159 (9)	0.0178 (9)	0.0007 (7)	0.0006 (7)	0.0005 (7)
C17B	0.0261 (10)	0.0240 (11)	0.0158 (9)	0.0009 (8)	-0.0028 (7)	0.0017 (8)
C18B	0.0253 (10)	0.0233 (11)	0.0178 (9)	0.0051 (8)	0.0037 (7)	0.0071 (8)
C19B	0.0180 (8)	0.0164 (10)	0.0257 (10)	0.0001 (7)	0.0074 (7)	0.0020 (8)
C20B	0.0128 (8)	0.0194 (10)	0.0211 (9)	-0.0014 (7)	0.0022 (7)	0.0005 (7)

Geometric parameters (Å, °)

C11A—C16A	1.7280 (19)	C11B—C16B	1.730 (2)
C12A—C18A	1.7290 (19)	C12B—C18B	1.7255 (19)
C13A—C19A	1.727 (2)	C13B—C19B	1.725 (2)
O1A—C14A	1.230 (2)	O1B—C14B	1.236 (2)
N1A—C14A	1.347 (2)	N1B—C14B	1.349 (2)
N1A—C15A	1.422 (2)	N1B—C15B	1.417 (2)
N1A—H1NA	0.78 (2)	N1B—H1NB	0.84 (2)
C1A—C6A	1.387 (3)	C1B—C2B	1.390 (3)
C1A—C2A	1.392 (3)	C1B—C6B	1.391 (3)
C1A—H1AA	0.9500	C1B—H1BA	0.9500
C2A—C3A	1.380 (3)	C2B—C3B	1.373 (4)
C2A—H2AA	0.9500	C2B—H2BA	0.9500
C3A—C4A	1.389 (3)	C3B—C4B	1.371 (4)
C3A—H3AA	0.9500	C3B—H3BA	0.9500
C4A—C5A	1.387 (3)	C4B—C5B	1.386 (3)
C4A—H4AA	0.9500	C4B—H4BA	0.9500
C5A—C6A	1.398 (3)	C5B—C6B	1.383 (3)
C5A—H5AA	0.9500	C5B—H5BA	0.9500
C6A—C7A	1.527 (2)	C6B—C7B	1.515 (3)
C7A—C8A	1.525 (2)	C7B—C14B	1.525 (2)
C7A—C14A	1.531 (2)	C7B—C8B	1.530 (2)
C7A—H7AA	1.0000	C7B—H7BA	1.0000
C8A—C13A	1.392 (3)	C8B—C13B	1.389 (3)
C8A—C9A	1.397 (3)	C8B—C9B	1.391 (3)
C9A—C10A	1.395 (3)	C9B—C10B	1.394 (3)
C9A—H9AA	0.9500	C9B—H9BA	0.9500
C10A—C11A	1.383 (3)	C10B—C11B	1.377 (4)
C10A—H10A	0.9500	C10B—H10B	0.9500
C11A—C12A	1.376 (3)	C11B—C12B	1.385 (4)
C11A—H11A	0.9500	C11B—H11B	0.9500
C12A—C13A	1.394 (3)	C12B—C13B	1.385 (3)

C12A—H12A	0.9500	C12B—H12B	0.9500
C13A—H13A	0.9500	C13B—H13B	0.9500
C15A—C20A	1.393 (3)	C15B—C20B	1.389 (3)
C15A—C16A	1.396 (2)	C15B—C16B	1.391 (2)
C16A—C17A	1.389 (3)	C16B—C17B	1.387 (3)
C17A—C18A	1.382 (3)	C17B—C18B	1.384 (3)
C17A—H17A	0.9500	C17B—H17B	0.9500
C18A—C19A	1.392 (3)	C18B—C19B	1.389 (3)
C19A—C20A	1.392 (3)	C19B—C20B	1.386 (3)
C20A—H20A	0.9500	C20B—H20B	0.9500
C14A—N1A—C15A	122.86 (14)	C14B—N1B—C15B	121.26 (15)
C14A—N1A—H1NA	121.7 (17)	C14B—N1B—H1NB	118.6 (15)
C15A—N1A—H1NA	113.9 (17)	C15B—N1B—H1NB	117.9 (15)
C6A—C1A—C2A	120.89 (18)	C2B—C1B—C6B	120.5 (2)
C6A—C1A—H1AA	119.6	C2B—C1B—H1BA	119.7
C2A—C1A—H1AA	119.6	C6B—C1B—H1BA	119.7
C3A—C2A—C1A	120.80 (19)	C3B—C2B—C1B	119.9 (2)
C3A—C2A—H2AA	119.6	C3B—C2B—H2BA	120.0
C1A—C2A—H2AA	119.6	C1B—C2B—H2BA	120.0
C2A—C3A—C4A	118.83 (19)	C4B—C3B—C2B	120.3 (2)
C2A—C3A—H3AA	120.6	C4B—C3B—H3BA	119.9
C4A—C3A—H3AA	120.6	C2B—C3B—H3BA	119.9
C5A—C4A—C3A	120.55 (19)	C3B—C4B—C5B	119.8 (2)
C5A—C4A—H4AA	119.7	C3B—C4B—H4BA	120.1
C3A—C4A—H4AA	119.7	C5B—C4B—H4BA	120.1
C4A—C5A—C6A	120.85 (18)	C6B—C5B—C4B	121.1 (2)
C4A—C5A—H5AA	119.6	C6B—C5B—H5BA	119.4
C6A—C5A—H5AA	119.6	C4B—C5B—H5BA	119.4
C1A—C6A—C5A	118.08 (18)	C5B—C6B—C1B	118.3 (2)
C1A—C6A—C7A	123.08 (16)	C5B—C6B—C7B	118.50 (18)
C5A—C6A—C7A	118.76 (16)	C1B—C6B—C7B	123.21 (17)
C8A—C7A—C6A	113.98 (14)	C6B—C7B—C14B	111.80 (15)
C8A—C7A—C14A	107.78 (14)	C6B—C7B—C8B	114.76 (15)
C6A—C7A—C14A	112.10 (14)	C14B—C7B—C8B	108.43 (14)
C8A—C7A—H7AA	107.6	C6B—C7B—H7BA	107.2
C6A—C7A—H7AA	107.6	C14B—C7B—H7BA	107.2
C14A—C7A—H7AA	107.6	C8B—C7B—H7BA	107.2
C13A—C8A—C9A	118.95 (18)	C13B—C8B—C9B	119.05 (19)
C13A—C8A—C7A	119.73 (16)	C13B—C8B—C7B	118.58 (17)
C9A—C8A—C7A	121.23 (16)	C9B—C8B—C7B	122.36 (18)
C10A—C9A—C8A	119.9 (2)	C8B—C9B—C10B	119.9 (2)
C10A—C9A—H9AA	120.0	C8B—C9B—H9BA	120.1
C8A—C9A—H9AA	120.0	C10B—C9B—H9BA	120.1
C11A—C10A—C9A	120.4 (2)	C11B—C10B—C9B	120.7 (2)
C11A—C10A—H10A	119.8	C11B—C10B—H10B	119.7
C9A—C10A—H10A	119.8	C9B—C10B—H10B	119.7
C12A—C11A—C10A	120.1 (2)	C10B—C11B—C12B	119.6 (2)

C12A—C11A—H11A	120.0	C10B—C11B—H11B	120.2
C10A—C11A—H11A	120.0	C12B—C11B—H11B	120.2
C11A—C12A—C13A	120.1 (2)	C13B—C12B—C11B	120.1 (2)
C11A—C12A—H12A	120.0	C13B—C12B—H12B	120.0
C13A—C12A—H12A	120.0	C11B—C12B—H12B	120.0
C8A—C13A—C12A	120.6 (2)	C12B—C13B—C8B	120.7 (2)
C8A—C13A—H13A	119.7	C12B—C13B—H13B	119.6
C12A—C13A—H13A	119.7	C8B—C13B—H13B	119.6
O1A—C14A—N1A	122.55 (16)	O1B—C14B—N1B	122.29 (16)
O1A—C14A—C7A	121.42 (15)	O1B—C14B—C7B	122.34 (15)
N1A—C14A—C7A	116.03 (14)	N1B—C14B—C7B	115.37 (14)
C20A—C15A—C16A	118.39 (16)	C20B—C15B—C16B	119.08 (17)
C20A—C15A—N1A	118.89 (16)	C20B—C15B—N1B	118.45 (16)
C16A—C15A—N1A	122.68 (16)	C16B—C15B—N1B	122.46 (17)
C17A—C16A—C15A	121.05 (17)	C17B—C16B—C15B	120.31 (18)
C17A—C16A—C11A	117.62 (14)	C17B—C16B—C11B	119.22 (15)
C15A—C16A—C11A	121.32 (14)	C15B—C16B—C11B	120.47 (14)
C18A—C17A—C16A	119.91 (18)	C18B—C17B—C16B	120.06 (18)
C18A—C17A—H17A	120.0	C18B—C17B—H17B	120.0
C16A—C17A—H17A	120.0	C16B—C17B—H17B	120.0
C17A—C18A—C19A	119.95 (17)	C17B—C18B—C19B	120.09 (17)
C17A—C18A—C12A	118.41 (15)	C17B—C18B—C12B	118.85 (15)
C19A—C18A—C12A	121.63 (15)	C19B—C18B—C12B	121.06 (16)
C20A—C19A—C18A	119.87 (18)	C20B—C19B—C18B	119.56 (18)
C20A—C19A—C13A	118.87 (15)	C20B—C19B—C13B	118.63 (15)
C18A—C19A—C13A	121.26 (15)	C18B—C19B—C13B	121.79 (15)
C19A—C20A—C15A	120.80 (17)	C19B—C20B—C15B	120.78 (18)
C19A—C20A—H20A	119.6	C19B—C20B—H20B	119.6
C15A—C20A—H20A	119.6	C15B—C20B—H20B	119.6
C6A—C1A—C2A—C3A	-0.4 (3)	C6B—C1B—C2B—C3B	-0.2 (3)
C1A—C2A—C3A—C4A	-0.2 (3)	C1B—C2B—C3B—C4B	-0.4 (3)
C2A—C3A—C4A—C5A	0.5 (3)	C2B—C3B—C4B—C5B	0.6 (4)
C3A—C4A—C5A—C6A	-0.1 (3)	C3B—C4B—C5B—C6B	-0.2 (4)
C2A—C1A—C6A—C5A	0.8 (3)	C4B—C5B—C6B—C1B	-0.4 (3)
C2A—C1A—C6A—C7A	177.36 (17)	C4B—C5B—C6B—C7B	178.9 (2)
C4A—C5A—C6A—C1A	-0.5 (3)	C2B—C1B—C6B—C5B	0.6 (3)
C4A—C5A—C6A—C7A	-177.25 (17)	C2B—C1B—C6B—C7B	-178.70 (18)
C1A—C6A—C7A—C8A	134.20 (17)	C5B—C6B—C7B—C14B	150.94 (17)
C5A—C6A—C7A—C8A	-49.2 (2)	C1B—C6B—C7B—C14B	-29.8 (2)
C1A—C6A—C7A—C14A	11.4 (2)	C5B—C6B—C7B—C8B	-85.0 (2)
C5A—C6A—C7A—C14A	-172.01 (16)	C1B—C6B—C7B—C8B	94.3 (2)
C6A—C7A—C8A—C13A	134.90 (17)	C6B—C7B—C8B—C13B	172.77 (17)
C14A—C7A—C8A—C13A	-99.99 (19)	C14B—C7B—C8B—C13B	-61.4 (2)
C6A—C7A—C8A—C9A	-48.6 (2)	C6B—C7B—C8B—C9B	-8.2 (2)
C14A—C7A—C8A—C9A	76.5 (2)	C14B—C7B—C8B—C9B	117.61 (18)
C13A—C8A—C9A—C10A	1.4 (3)	C13B—C8B—C9B—C10B	-1.3 (3)
C7A—C8A—C9A—C10A	-175.14 (17)	C7B—C8B—C9B—C10B	179.69 (17)

C8A—C9A—C10A—C11A	-1.0 (3)	C8B—C9B—C10B—C11B	0.8 (3)
C9A—C10A—C11A—C12A	-0.5 (3)	C9B—C10B—C11B—C12B	0.3 (3)
C10A—C11A—C12A—C13A	1.4 (3)	C10B—C11B—C12B—C13B	-0.9 (3)
C9A—C8A—C13A—C12A	-0.4 (3)	C11B—C12B—C13B—C8B	0.4 (3)
C7A—C8A—C13A—C12A	176.15 (18)	C9B—C8B—C13B—C12B	0.7 (3)
C11A—C12A—C13A—C8A	-1.0 (3)	C7B—C8B—C13B—C12B	179.76 (18)
C15A—N1A—C14A—O1A	3.2 (3)	C15B—N1B—C14B—O1B	6.1 (3)
C15A—N1A—C14A—C7A	-175.56 (16)	C15B—N1B—C14B—C7B	-173.02 (16)
C8A—C7A—C14A—O1A	-53.7 (2)	C6B—C7B—C14B—O1B	77.7 (2)
C6A—C7A—C14A—O1A	72.6 (2)	C8B—C7B—C14B—O1B	-49.8 (2)
C8A—C7A—C14A—N1A	125.16 (16)	C6B—C7B—C14B—N1B	-103.22 (18)
C6A—C7A—C14A—N1A	-108.62 (17)	C8B—C7B—C14B—N1B	129.28 (16)
C14A—N1A—C15A—C20A	113.08 (19)	C14B—N1B—C15B—C20B	110.5 (2)
C14A—N1A—C15A—C16A	-69.2 (2)	C14B—N1B—C15B—C16B	-68.5 (2)
C20A—C15A—C16A—C17A	0.6 (3)	C20B—C15B—C16B—C17B	-3.6 (3)
N1A—C15A—C16A—C17A	-177.11 (16)	N1B—C15B—C16B—C17B	175.38 (17)
C20A—C15A—C16A—C11A	179.03 (13)	C20B—C15B—C16B—C11B	176.16 (14)
N1A—C15A—C16A—C11A	1.3 (2)	N1B—C15B—C16B—C11B	-4.8 (2)
C15A—C16A—C17A—C18A	0.9 (3)	C15B—C16B—C17B—C18B	1.2 (3)
C11A—C16A—C17A—C18A	-177.56 (14)	C11B—C16B—C17B—C18B	-178.54 (15)
C16A—C17A—C18A—C19A	-2.0 (3)	C16B—C17B—C18B—C19B	2.1 (3)
C16A—C17A—C18A—C12A	176.97 (14)	C16B—C17B—C18B—C12B	-176.94 (15)
C17A—C18A—C19A—C20A	1.5 (3)	C17B—C18B—C19B—C20B	-3.1 (3)
C12A—C18A—C19A—C20A	-177.41 (14)	C12B—C18B—C19B—C20B	175.99 (14)
C17A—C18A—C19A—C13A	-179.15 (14)	C17B—C18B—C19B—C13B	178.72 (15)
C12A—C18A—C19A—C13A	2.0 (2)	C12B—C18B—C19B—C13B	-2.2 (2)
C18A—C19A—C20A—C15A	0.1 (3)	C18B—C19B—C20B—C15B	0.6 (3)
C13A—C19A—C20A—C15A	-179.32 (13)	C13B—C19B—C20B—C15B	178.91 (14)
C16A—C15A—C20A—C19A	-1.1 (3)	C16B—C15B—C20B—C19B	2.7 (3)
N1A—C15A—C20A—C19A	176.72 (16)	N1B—C15B—C20B—C19B	-176.36 (16)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1A—H1NA \cdots O1B ⁱ	0.78 (2)	2.09 (2)	2.8379 (19)	161 (2)
N1B—H1NB \cdots O1A	0.84 (2)	1.94 (2)	2.7684 (19)	168 (2)
C7A—H7AA \cdots O1B ⁱ	1.00	2.33	3.234 (2)	151
C1B—H1BA \cdots O1B	0.95	2.48	3.116 (3)	125
C3B—H3BA \cdots O1B ⁱⁱ	0.95	2.42	3.368 (3)	172
C12B—H12B \cdots C12B ⁱⁱⁱ	0.95	2.82	3.641 (3)	145
C7B—H7BA \cdots O1A	1.00	2.46	3.341 (2)	147

Symmetry codes: (i) $x+1/2, y, -z+1/2$; (ii) $-x, y-1/2, -z+1/2$; (iii) $x, -y+5/2, z+1/2$.