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1-[5-(2-Chlorophenyl)-3-(4-methylphenyl)-4,5-dihydro-1*H*-pyrazol-1-yl]ethan-1-one

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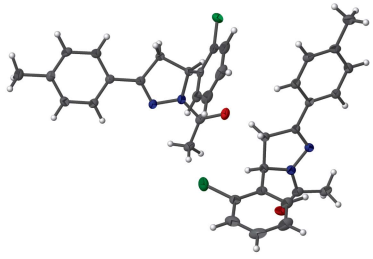
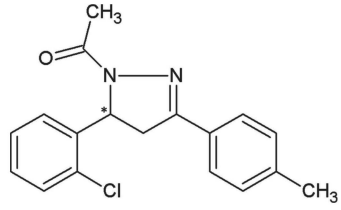
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{18}H_{17}ClN_2O$, crystallized with two independent molecules (the *S* and *R* enantiomers) in the asymmetric unit. The molecules are V-shaped with the two aromatic rings inclined to one another by 78.78 (11) and 81.23 (11)°. In the crystal, molecules are linked *via* C—H···O hydrogen bonds, forming chains along the *c*-axis direction. The chains are linked *via* C—H···π interactions, forming a three-dimensional framework. The crystal structure was refined as a two-component twin.

3D view



Chemical scheme



Structure description

Pyrazoline derivatives are well known for their versatile pharmacological activities (Sarojini *et al.*, 2010; Samshuddin *et al.*, 2012). Many 1,3,5-triaryl-2-pyrazolines have a variety of industrial applications; used as scintillation solutes (Wiley *et al.*, 1958) and as fluorescent agents (Zhi-Yun *et al.*, 1999). In view of the importance of pyrazolines the title compound, a new *N*-acetyl substituted pyrazoline derivative, was prepared by the condensation of (2*E*)-3-(2-chlorophenyl)-1-(4-methylphenyl)prop-2-en-1-one and hydrazine hydrate in the presence of acetic acid.

The title compound, Fig. 1, crystallized with two independent molecules (*A* and *B*: the *S* and *R* enantiomers, respectively) in the asymmetric unit. The pyrazole ring in molecule *A* has an envelope conformation with the chiral C atom, C7*A*, as the flap. In molecule *B* the pyrazole ring has a twist conformation on the CH—CH_2 (C7*B*—C8*B*) bond. Their mean planes are inclined to the 4-methylbenzene ring by 5.65 (12)° in *A* and by 8.99 (12)° in *B*. The two aromatic rings are inclined to one another by 78.78 (11)° in molecule *A* and by 81.23 (11)° in molecule *B*.

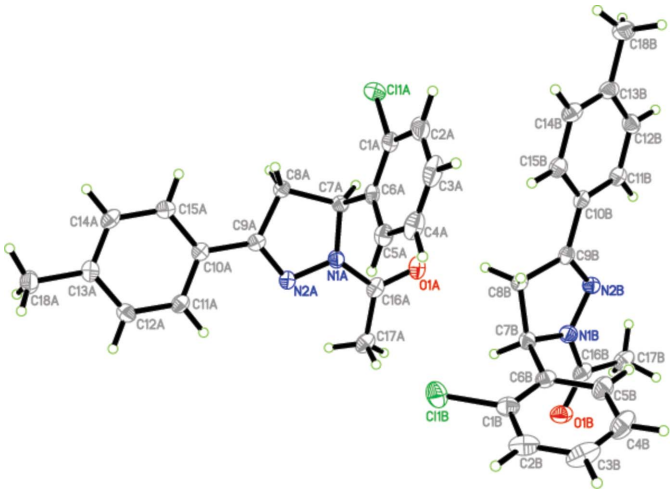


Figure 1
The molecular structure of the title compound, showin the atom labelling and 50% probability displacement ellipsoids.

In the crystal, molecules are linked *via* C—H···O hydrogen bonds, forming chains along [001]; see Table 1 and Fig. 2. The chains are linked *via* C—H···π interactions forming a three-dimensional framework (Table 1).

Synthesis and crystallization

A mixture of (2*E*)-3-(2-chlorophenyl)-1-(4-methylphenyl)prop-2-en-1-one (2.56 g, 0.01 mol) and hydrazine hydrate (1 ml) in 30 ml acetic acid was refluxed for 8 h. The reaction mixture was cooled and poured into 100 ml ice-cold water. The precipitate was collected by filtration and purified by recrystallization from ethanol. Single crystals were grown from ethanol by slow evaporation (yield 70%; m.p. 409–412 K).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal structure was refined as a 2-component twin [180° rotation about the *b** axis; BASF = 0.431 (1)].

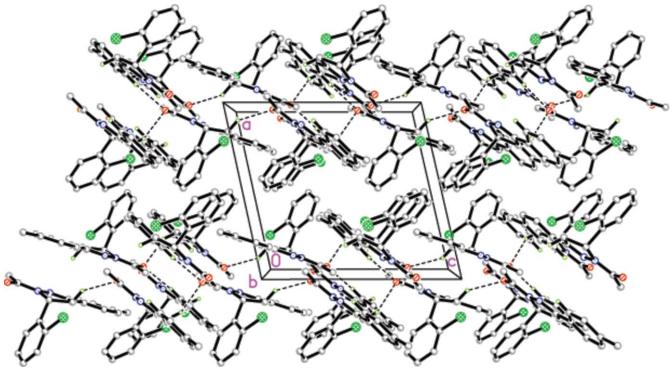


Figure 2
The crystal packing of the title compound viewed along the *b* axis. Hydrogen bonds are shown as dashed lines (see Table 1).

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

*Cg*3 and *Cg*6 are the centroids of rings C10*A*–C15*A* and C10*B*–C15*B*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8*A*—H8*AB*···O1*B*^{i}	0.99	2.48	3.362 (3)	149
C11*B*—H11*B*···O1*A*^{ii}	0.95	2.56	3.458 (3)	159
C8*B*—H8*BA*···O1*A*	0.99	2.42	3.319 (3)	151
C3*A*—H3*AA*···*Cg*6^{iii}	0.95	2.69	3.550 (3)	151
C3*B*—H3*BA*···*Cg*3^{iv}	0.95	2.95	3.616 (3)	128

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

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{17}ClN_2O$
M_r	312.79
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	11.0767 (12), 12.0670 (13), 12.1600 (13)
α, β, γ (°)	90.825 (2), 102.5614 (19), 95.142 (2)
V (Å^3)	1579.1 (3)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.25
Crystal size (mm)	0.49 × 0.31 × 0.29
Data collection	
Diffractometer	Bruker *APEX* DUO CCD area-detector diffractometer
Absorption correction	Multi-scan (*TWINABS*; Bruker, 2009)
T_{min}, T_{max}	0.711, 0.857
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5665, 5665, 5334
R_{int}	?
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.040, 0.119, 1.10
No. of reflections	5665
No. of parameters	402
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.35

Computer programs: *APEX2* (Bruker, 2009), *SAINT* (Bruker, 2009), *SHELXS2013* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2016). **1**, x152460 [doi:10.1107/S2414314615024608]

1-[5-(2-Chlorophenyl)-3-(4-methylphenyl)-4,5-dihydro-1*H*-pyrazol-1-yl]ethan-1-one

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Crystal data

$C_{18}H_{17}ClN_2O$
M_r = 312.79
Triclinic, $P\overline{1}$
a = 11.0767 (12) Å
b = 12.0670 (13) Å
c = 12.1600 (13) Å
α = 90.825 (2)°
β = 102.5614 (19)°
γ = 95.142 (2)°
V = 1579.1 (3) Å^3
Z = 4
$F(000)$ = 656
D_x = 1.316 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9954 reflections
θ = 2.3–25.1°
μ = 0.25 mm^{-1}
T = 100 K
Block, colourless
0.49 × 0.31 × 0.29 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*TWINABS*; Bruker, 2009)
T_{min} = 0.711, T_{max} = 0.857
5665 measured reflections
5665 independent reflections
5334 reflections with $I > 2\sigma(I)$
θ_{max} = 25.1°, θ_{min} = 1.7°
h = −13→12
k = −14→14
l = 0→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.119
S = 1.10
5665 reflections
402 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0832P)^2 + 0.2751P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refined as a 2-component twin

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1A	0.21908 (7)	0.08540 (5)	0.04400 (6)	0.03442 (17)
O1A	0.03134 (16)	0.25816 (14)	0.32387 (14)	0.0274 (4)
N1A	0.09059 (18)	0.37602 (16)	0.20123 (16)	0.0204 (4)
N2A	0.10951 (17)	0.48329 (16)	0.16358 (16)	0.0187 (4)
C1A	0.3041 (2)	0.1604 (2)	0.1639 (2)	0.0240 (5)
C2A	0.4170 (3)	0.1255 (2)	0.2180 (2)	0.0345 (6)
H2AA	0.4466	0.0610	0.1912	0.041*
C3A	0.4860 (2)	0.1861 (3)	0.3118 (2)	0.0350 (6)
H3AA	0.5632	0.1628	0.3503	0.042*
C4A	0.4431 (2)	0.2799 (2)	0.3495 (2)	0.0305 (6)
H4AA	0.4911	0.3217	0.4134	0.037*
C5A	0.3302 (2)	0.3133 (2)	0.2942 (2)	0.0240 (5)
H5AA	0.3016	0.3782	0.3210	0.029*
C6A	0.2577 (2)	0.25441 (18)	0.20064 (19)	0.0195 (5)
C7A	0.1359 (2)	0.29186 (19)	0.13625 (19)	0.0194 (5)
H7AA	0.0720	0.2269	0.1139	0.023*
C8A	0.1540 (2)	0.35784 (18)	0.03170 (19)	0.0202 (5)
H8AA	0.2357	0.3484	0.0140	0.024*
H8AB	0.0873	0.3351	−0.0353	0.024*
C9A	0.14683 (19)	0.47560 (19)	0.07111 (18)	0.0178 (4)
C10A	0.17624 (19)	0.57493 (18)	0.01095 (18)	0.0176 (4)
C11A	0.1686 (2)	0.68142 (19)	0.05564 (19)	0.0208 (5)
H11A	0.1440	0.6891	0.1253	0.025*
C12A	0.1967 (2)	0.7746 (2)	−0.0014 (2)	0.0238 (5)
H12A	0.1900	0.8461	0.0292	0.029*
C13A	0.2347 (2)	0.7666 (2)	−0.1027 (2)	0.0220 (5)
C14A	0.2435 (2)	0.6615 (2)	−0.1464 (2)	0.0229 (5)
H14A	0.2698	0.6544	−0.2153	0.027*
C15A	0.2146 (2)	0.56628 (19)	−0.09058 (19)	0.0211 (5)
H15A	0.2209	0.4949	−0.1218	0.025*
C16A	0.0419 (2)	0.3539 (2)	0.2927 (2)	0.0222 (5)
C17A	0.0064 (2)	0.4513 (2)	0.3527 (2)	0.0274 (5)
H17A	−0.0123	0.5112	0.2999	0.041*
H17B	0.0754	0.4780	0.4151	0.041*
H17C	−0.0671	0.4283	0.3824	0.041*
C18A	0.2599 (3)	0.8699 (2)	−0.1655 (2)	0.0310 (6)
H18A	0.3182	0.9237	−0.1146	0.047*
H18B	0.1818	0.9030	−0.1936	0.047*
H18C	0.2959	0.8503	−0.2291	0.047*
Cl1B	0.31200 (6)	0.46911 (5)	0.58780 (6)	0.03452 (17)
O1B	0.02652 (17)	0.27178 (15)	0.76408 (14)	0.0297 (4)
N1B	0.11108 (19)	0.15285 (16)	0.66688 (16)	0.0213 (4)
N2B	0.12585 (17)	0.04611 (15)	0.63221 (16)	0.0194 (4)

C1B	0.3553 (2)	0.3952 (2)	0.7108 (2)	0.0249 (5)
C2B	0.4501 (2)	0.4432 (2)	0.7954 (2)	0.0318 (6)
H2BA	0.4881	0.5156	0.7877	0.038*
C3B	0.4892 (2)	0.3849 (3)	0.8915 (2)	0.0380 (7)
H3BA	0.5547	0.4169	0.9502	0.046*
C4B	0.4327 (2)	0.2796 (3)	0.9023 (2)	0.0365 (6)
H4BA	0.4602	0.2390	0.9679	0.044*
C5B	0.3363 (2)	0.2337 (2)	0.8175 (2)	0.0292 (5)
H5BA	0.2976	0.1618	0.8259	0.035*
C6B	0.2944 (2)	0.2914 (2)	0.71936 (19)	0.0221 (5)
C7B	0.1899 (2)	0.23941 (19)	0.62557 (19)	0.0206 (5)
H7BA	0.1388	0.2980	0.5879	0.025*
C8B	0.2386 (2)	0.17185 (19)	0.53747 (19)	0.0222 (5)
H8BA	0.1997	0.1905	0.4595	0.027*
H8BB	0.3300	0.1848	0.5488	0.027*
C9B	0.1987 (2)	0.05402 (18)	0.56220 (18)	0.0183 (5)
C10B	0.2338 (2)	−0.04471 (19)	0.51034 (19)	0.0194 (5)
C11B	0.1761 (2)	−0.15102 (19)	0.52063 (19)	0.0202 (5)
H11B	0.1133	−0.1601	0.5629	0.024*
C12B	0.2099 (2)	−0.2424 (2)	0.4697 (2)	0.0243 (5)
H12B	0.1704	−0.3140	0.4779	0.029*
C13B	0.3016 (2)	−0.2322 (2)	0.4060 (2)	0.0239 (5)
C14B	0.3578 (2)	−0.1270 (2)	0.3965 (2)	0.0245 (5)
H14B	0.4204	−0.1181	0.3540	0.029*
C15B	0.3254 (2)	−0.0342 (2)	0.44718 (19)	0.0219 (5)
H15B	0.3655	0.0371	0.4390	0.026*
C16B	0.0340 (2)	0.1753 (2)	0.73584 (19)	0.0235 (5)
C17B	−0.0383 (2)	0.0777 (2)	0.7745 (2)	0.0286 (5)
H17D	−0.0357	0.0114	0.7278	0.043*
H17E	−0.1248	0.0938	0.7674	0.043*
H17F	−0.0017	0.0643	0.8535	0.043*
C18B	0.3362 (3)	−0.3328 (2)	0.3498 (2)	0.0321 (6)
H18D	0.2606	−0.3786	0.3121	0.048*
H18E	0.3865	−0.3764	0.4066	0.048*
H18F	0.3841	−0.3088	0.2939	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1A	0.0516 (4)	0.0218 (3)	0.0306 (3)	0.0038 (3)	0.0108 (3)	−0.0039 (2)
O1A	0.0261 (9)	0.0289 (9)	0.0274 (9)	0.0012 (7)	0.0065 (7)	0.0094 (7)
N1A	0.0215 (10)	0.0197 (9)	0.0215 (10)	0.0038 (8)	0.0071 (8)	0.0035 (8)
N2A	0.0166 (9)	0.0203 (9)	0.0193 (9)	0.0019 (7)	0.0039 (7)	0.0031 (7)
C1A	0.0285 (12)	0.0234 (12)	0.0217 (12)	0.0027 (10)	0.0089 (10)	0.0059 (9)
C2A	0.0416 (16)	0.0355 (14)	0.0361 (15)	0.0198 (12)	0.0221 (13)	0.0154 (12)
C3A	0.0187 (12)	0.0581 (18)	0.0316 (14)	0.0114 (12)	0.0082 (10)	0.0222 (13)
C4A	0.0204 (12)	0.0435 (15)	0.0239 (12)	−0.0046 (11)	−0.0002 (10)	0.0084 (11)
C5A	0.0199 (12)	0.0261 (12)	0.0249 (12)	−0.0029 (9)	0.0045 (9)	0.0044 (9)

C6A	0.0199 (11)	0.0190 (11)	0.0209 (11)	−0.0014 (9)	0.0081 (9)	0.0062 (9)
C7A	0.0208 (11)	0.0182 (11)	0.0191 (11)	0.0017 (9)	0.0039 (9)	0.0010 (8)
C8A	0.0224 (12)	0.0206 (11)	0.0180 (11)	0.0035 (9)	0.0044 (9)	0.0009 (9)
C9A	0.0120 (10)	0.0233 (11)	0.0164 (10)	0.0030 (9)	−0.0006 (8)	−0.0002 (9)
C10A	0.0116 (10)	0.0227 (11)	0.0179 (11)	0.0022 (8)	0.0013 (8)	0.0011 (9)
C11A	0.0182 (11)	0.0264 (12)	0.0184 (11)	0.0029 (9)	0.0049 (9)	0.0016 (9)
C12A	0.0250 (12)	0.0198 (11)	0.0272 (12)	0.0037 (9)	0.0062 (10)	0.0004 (9)
C13A	0.0168 (11)	0.0251 (11)	0.0237 (11)	0.0019 (9)	0.0034 (9)	0.0051 (9)
C14A	0.0187 (11)	0.0332 (13)	0.0179 (11)	0.0040 (9)	0.0060 (9)	0.0011 (9)
C15A	0.0182 (11)	0.0242 (11)	0.0197 (11)	0.0038 (9)	0.0013 (9)	−0.0009 (9)
C16A	0.0146 (11)	0.0321 (13)	0.0197 (11)	0.0024 (9)	0.0028 (9)	0.0044 (10)
C17A	0.0258 (12)	0.0362 (14)	0.0217 (12)	0.0028 (10)	0.0087 (10)	0.0014 (10)
C18A	0.0360 (15)	0.0280 (13)	0.0325 (14)	0.0045 (11)	0.0139 (12)	0.0080 (11)
Cl1B	0.0337 (3)	0.0277 (3)	0.0408 (4)	−0.0019 (3)	0.0069 (3)	0.0074 (3)
O1B	0.0291 (9)	0.0328 (10)	0.0269 (9)	0.0100 (8)	0.0032 (7)	−0.0061 (7)
N1B	0.0205 (10)	0.0215 (10)	0.0223 (10)	0.0029 (8)	0.0053 (8)	0.0004 (8)
N2B	0.0187 (9)	0.0198 (9)	0.0196 (9)	0.0019 (7)	0.0038 (8)	−0.0006 (7)
C1B	0.0217 (12)	0.0279 (12)	0.0272 (13)	0.0030 (10)	0.0097 (10)	−0.0031 (10)
C2B	0.0185 (12)	0.0384 (15)	0.0388 (15)	−0.0025 (11)	0.0099 (11)	−0.0140 (12)
C3B	0.0151 (12)	0.066 (2)	0.0313 (15)	−0.0015 (12)	0.0050 (11)	−0.0158 (13)
C4B	0.0229 (13)	0.0617 (19)	0.0241 (13)	0.0077 (13)	0.0014 (10)	0.0039 (12)
C5B	0.0245 (12)	0.0385 (14)	0.0238 (12)	0.0054 (11)	0.0030 (10)	0.0025 (11)
C6B	0.0200 (12)	0.0265 (12)	0.0200 (11)	0.0039 (10)	0.0046 (9)	−0.0025 (9)
C7B	0.0211 (11)	0.0206 (11)	0.0195 (11)	0.0023 (9)	0.0027 (9)	0.0012 (9)
C8B	0.0274 (12)	0.0214 (11)	0.0181 (11)	0.0010 (9)	0.0061 (9)	0.0014 (9)
C9B	0.0161 (11)	0.0216 (11)	0.0159 (10)	0.0014 (9)	0.0009 (8)	0.0023 (8)
C10B	0.0183 (11)	0.0242 (11)	0.0152 (10)	0.0022 (9)	0.0028 (8)	0.0025 (9)
C11B	0.0170 (11)	0.0239 (11)	0.0187 (11)	0.0005 (9)	0.0025 (9)	0.0016 (9)
C12B	0.0266 (12)	0.0204 (11)	0.0238 (12)	0.0009 (9)	0.0013 (10)	0.0014 (9)
C13B	0.0244 (12)	0.0286 (12)	0.0173 (11)	0.0072 (10)	−0.0001 (9)	−0.0030 (9)
C14B	0.0215 (12)	0.0328 (13)	0.0200 (11)	0.0032 (10)	0.0062 (9)	−0.0008 (10)
C15B	0.0199 (11)	0.0255 (11)	0.0204 (11)	0.0005 (9)	0.0052 (9)	0.0023 (9)
C16B	0.0170 (11)	0.0342 (13)	0.0182 (10)	0.0049 (10)	0.0005 (9)	−0.0008 (10)
C17B	0.0218 (12)	0.0425 (14)	0.0229 (12)	0.0027 (11)	0.0080 (10)	−0.0001 (11)
C18B	0.0371 (15)	0.0338 (14)	0.0245 (13)	0.0074 (12)	0.0036 (11)	−0.0043 (11)

Geometric parameters (Å, º)

Cl1A—C1A	1.744 (3)	Cl1B—C1B	1.751 (3)
O1A—C16A	1.225 (3)	O1B—C16B	1.225 (3)
N1A—C16A	1.357 (3)	N1B—C16B	1.361 (3)
N1A—N2A	1.393 (3)	N1B—N2B	1.384 (3)
N1A—C7A	1.466 (3)	N1B—C7B	1.466 (3)
N2A—C9A	1.285 (3)	N2B—C9B	1.293 (3)
C1A—C2A	1.385 (4)	C1B—C2B	1.379 (4)
C1A—C6A	1.394 (3)	C1B—C6B	1.385 (4)
C2A—C3A	1.385 (4)	C2B—C3B	1.380 (4)
C2A—H2AA	0.9500	C2B—H2BA	0.9500

C3A—C4A	1.376 (4)	C3B—C4B	1.386 (4)
C3A—H3AA	0.9500	C3B—H3BA	0.9500
C4A—C5A	1.383 (4)	C4B—C5B	1.381 (4)
C4A—H4AA	0.9500	C4B—H4BA	0.9500
C5A—C6A	1.386 (3)	C5B—C6B	1.401 (3)
C5A—H5AA	0.9500	C5B—H5BA	0.9500
C6A—C7A	1.515 (3)	C6B—C7B	1.519 (3)
C7A—C8A	1.550 (3)	C7B—C8B	1.551 (3)
C7A—H7AA	1.0000	C7B—H7BA	1.0000
C8A—C9A	1.508 (3)	C8B—C9B	1.505 (3)
C8A—H8AA	0.9900	C8B—H8BA	0.9900
C8A—H8AB	0.9900	C8B—H8BB	0.9900
C9A—C10A	1.462 (3)	C9B—C10B	1.462 (3)
C10A—C15A	1.396 (3)	C10B—C15B	1.397 (3)
C10A—C11A	1.405 (3)	C10B—C11B	1.401 (3)
C11A—C12A	1.377 (3)	C11B—C12B	1.377 (3)
C11A—H11A	0.9500	C11B—H11B	0.9500
C12A—C13A	1.390 (3)	C12B—C13B	1.403 (4)
C12A—H12A	0.9500	C12B—H12B	0.9500
C13A—C14A	1.388 (3)	C13B—C14B	1.381 (4)
C13A—C18A	1.508 (3)	C13B—C18B	1.504 (3)
C14A—C15A	1.391 (3)	C14B—C15B	1.383 (3)
C14A—H14A	0.9500	C14B—H14B	0.9500
C15A—H15A	0.9500	C15B—H15B	0.9500
C16A—C17A	1.501 (3)	C16B—C17B	1.503 (4)
C17A—H17A	0.9800	C17B—H17D	0.9800
C17A—H17B	0.9800	C17B—H17E	0.9800
C17A—H17C	0.9800	C17B—H17F	0.9800
C18A—H18A	0.9800	C18B—H18D	0.9800
C18A—H18B	0.9800	C18B—H18E	0.9800
C18A—H18C	0.9800	C18B—H18F	0.9800

C16A—N1A—N2A	122.91 (19)	C16B—N1B—N2B	123.3 (2)
C16A—N1A—C7A	124.13 (19)	C16B—N1B—C7B	123.1 (2)
N2A—N1A—C7A	112.85 (17)	N2B—N1B—C7B	113.53 (18)
C9A—N2A—N1A	107.83 (18)	C9B—N2B—N1B	107.86 (18)
C2A—C1A—C6A	122.2 (2)	C2B—C1B—C6B	122.6 (2)
C2A—C1A—Cl1A	118.7 (2)	C2B—C1B—Cl1B	118.1 (2)
C6A—C1A—Cl1A	119.08 (19)	C6B—C1B—Cl1B	119.29 (19)
C3A—C2A—C1A	118.9 (2)	C1B—C2B—C3B	119.2 (3)
C3A—C2A—H2AA	120.6	C1B—C2B—H2BA	120.4
C1A—C2A—H2AA	120.6	C3B—C2B—H2BA	120.4
C4A—C3A—C2A	120.2 (2)	C2B—C3B—C4B	120.0 (2)
C4A—C3A—H3AA	119.9	C2B—C3B—H3BA	120.0
C2A—C3A—H3AA	119.9	C4B—C3B—H3BA	120.0
C3A—C4A—C5A	120.0 (2)	C5B—C4B—C3B	119.9 (3)
C3A—C4A—H4AA	120.0	C5B—C4B—H4BA	120.0
C5A—C4A—H4AA	120.0	C3B—C4B—H4BA	120.0

C4A—C5A—C6A	121.7 (2)	C4B—C5B—C6B	121.3 (3)
C4A—C5A—H5AA	119.2	C4B—C5B—H5BA	119.4
C6A—C5A—H5AA	119.2	C6B—C5B—H5BA	119.4
C5A—C6A—C1A	117.0 (2)	C1B—C6B—C5B	116.9 (2)
C5A—C6A—C7A	122.5 (2)	C1B—C6B—C7B	122.1 (2)
C1A—C6A—C7A	120.4 (2)	C5B—C6B—C7B	120.9 (2)
N1A—C7A—C6A	111.47 (19)	N1B—C7B—C6B	111.94 (18)
N1A—C7A—C8A	101.24 (17)	N1B—C7B—C8B	101.23 (18)
C6A—C7A—C8A	111.26 (19)	C6B—C7B—C8B	112.36 (19)
N1A—C7A—H7AA	110.8	N1B—C7B—H7BA	110.3
C6A—C7A—H7AA	110.8	C6B—C7B—H7BA	110.3
C8A—C7A—H7AA	110.8	C8B—C7B—H7BA	110.3
C9A—C8A—C7A	101.45 (17)	C9B—C8B—C7B	101.85 (18)
C9A—C8A—H8AA	111.5	C9B—C8B—H8BA	111.4
C7A—C8A—H8AA	111.5	C7B—C8B—H8BA	111.4
C9A—C8A—H8AB	111.5	C9B—C8B—H8BB	111.4
C7A—C8A—H8AB	111.5	C7B—C8B—H8BB	111.4
H8AA—C8A—H8AB	109.3	H8BA—C8B—H8BB	109.3
N2A—C9A—C10A	121.0 (2)	N2B—C9B—C10B	121.5 (2)
N2A—C9A—C8A	114.3 (2)	N2B—C9B—C8B	114.06 (19)
C10A—C9A—C8A	124.68 (19)	C10B—C9B—C8B	124.4 (2)
C15A—C10A—C11A	118.7 (2)	C15B—C10B—C11B	118.4 (2)
C15A—C10A—C9A	120.9 (2)	C15B—C10B—C9B	120.1 (2)
C11A—C10A—C9A	120.4 (2)	C11B—C10B—C9B	121.5 (2)
C12A—C11A—C10A	120.1 (2)	C12B—C11B—C10B	120.2 (2)
C12A—C11A—H11A	120.0	C12B—C11B—H11B	119.9
C10A—C11A—H11A	120.0	C10B—C11B—H11B	119.9
C11A—C12A—C13A	121.6 (2)	C11B—C12B—C13B	121.5 (2)
C11A—C12A—H12A	119.2	C11B—C12B—H12B	119.3
C13A—C12A—H12A	119.2	C13B—C12B—H12B	119.3
C14A—C13A—C12A	118.5 (2)	C14B—C13B—C12B	117.7 (2)
C14A—C13A—C18A	121.2 (2)	C14B—C13B—C18B	121.5 (2)
C12A—C13A—C18A	120.3 (2)	C12B—C13B—C18B	120.7 (2)
C13A—C14A—C15A	120.9 (2)	C13B—C14B—C15B	121.7 (2)
C13A—C14A—H14A	119.6	C13B—C14B—H14B	119.2
C15A—C14A—H14A	119.6	C15B—C14B—H14B	119.2
C14A—C15A—C10A	120.4 (2)	C14B—C15B—C10B	120.5 (2)
C14A—C15A—H15A	119.8	C14B—C15B—H15B	119.8
C10A—C15A—H15A	119.8	C10B—C15B—H15B	119.8
O1A—C16A—N1A	119.9 (2)	O1B—C16B—N1B	119.8 (2)
O1A—C16A—C17A	123.2 (2)	O1B—C16B—C17B	123.0 (2)
N1A—C16A—C17A	116.9 (2)	N1B—C16B—C17B	117.2 (2)
C16A—C17A—H17A	109.5	C16B—C17B—H17D	109.5
C16A—C17A—H17B	109.5	C16B—C17B—H17E	109.5
H17A—C17A—H17B	109.5	H17D—C17B—H17E	109.5
C16A—C17A—H17C	109.5	C16B—C17B—H17F	109.5
H17A—C17A—H17C	109.5	H17D—C17B—H17F	109.5
H17B—C17A—H17C	109.5	H17E—C17B—H17F	109.5

C13A—C18A—H18A	109.5	C13B—C18B—H18D	109.5
C13A—C18A—H18B	109.5	C13B—C18B—H18E	109.5
H18A—C18A—H18B	109.5	H18D—C18B—H18E	109.5
C13A—C18A—H18C	109.5	C13B—C18B—H18F	109.5
H18A—C18A—H18C	109.5	H18D—C18B—H18F	109.5
H18B—C18A—H18C	109.5	H18E—C18B—H18F	109.5
C16A—N1A—N2A—C9A	−174.9 (2)	C16B—N1B—N2B—C9B	176.0 (2)
C7A—N1A—N2A—C9A	8.8 (2)	C7B—N1B—N2B—C9B	−6.2 (2)
C6A—C1A—C2A—C3A	0.0 (4)	C6B—C1B—C2B—C3B	1.9 (4)
Cl1A—C1A—C2A—C3A	178.68 (19)	Cl1B—C1B—C2B—C3B	−177.57 (19)
C1A—C2A—C3A—C4A	−0.6 (4)	C1B—C2B—C3B—C4B	−0.3 (4)
C2A—C3A—C4A—C5A	0.6 (4)	C2B—C3B—C4B—C5B	−0.8 (4)
C3A—C4A—C5A—C6A	0.0 (4)	C3B—C4B—C5B—C6B	0.5 (4)
C4A—C5A—C6A—C1A	−0.6 (3)	C2B—C1B—C6B—C5B	−2.2 (3)
C4A—C5A—C6A—C7A	−177.7 (2)	Cl1B—C1B—C6B—C5B	177.29 (18)
C2A—C1A—C6A—C5A	0.6 (3)	C2B—C1B—C6B—C7B	180.0 (2)
Cl1A—C1A—C6A—C5A	−178.08 (17)	Cl1B—C1B—C6B—C7B	−0.5 (3)
C2A—C1A—C6A—C7A	177.8 (2)	C4B—C5B—C6B—C1B	1.0 (4)
Cl1A—C1A—C6A—C7A	−0.9 (3)	C4B—C5B—C6B—C7B	178.8 (2)
C16A—N1A—C7A—C6A	−72.6 (3)	C16B—N1B—C7B—C6B	69.3 (3)
N2A—N1A—C7A—C6A	103.7 (2)	N2B—N1B—C7B—C6B	−108.6 (2)
C16A—N1A—C7A—C8A	169.0 (2)	C16B—N1B—C7B—C8B	−170.9 (2)
N2A—N1A—C7A—C8A	−14.7 (2)	N2B—N1B—C7B—C8B	11.3 (2)
C5A—C6A—C7A—N1A	−15.5 (3)	C1B—C6B—C7B—N1B	−159.0 (2)
C1A—C6A—C7A—N1A	167.55 (19)	C5B—C6B—C7B—N1B	23.2 (3)
C5A—C6A—C7A—C8A	96.8 (3)	C1B—C6B—C7B—C8B	87.8 (3)
C1A—C6A—C7A—C8A	−80.2 (3)	C5B—C6B—C7B—C8B	−89.9 (3)
N1A—C7A—C8A—C9A	14.0 (2)	N1B—C7B—C8B—C9B	−11.2 (2)
C6A—C7A—C8A—C9A	−104.6 (2)	C6B—C7B—C8B—C9B	108.4 (2)
N1A—N2A—C9A—C10A	−179.30 (19)	N1B—N2B—C9B—C10B	179.58 (19)
N1A—N2A—C9A—C8A	1.9 (2)	N1B—N2B—C9B—C8B	−2.4 (3)
C7A—C8A—C9A—N2A	−10.7 (2)	C7B—C8B—C9B—N2B	9.1 (3)
C7A—C8A—C9A—C10A	170.6 (2)	C7B—C8B—C9B—C10B	−173.0 (2)
N2A—C9A—C10A—C15A	−178.8 (2)	N2B—C9B—C10B—C15B	−171.4 (2)
C8A—C9A—C10A—C15A	−0.1 (3)	C8B—C9B—C10B—C15B	10.8 (3)
N2A—C9A—C10A—C11A	2.4 (3)	N2B—C9B—C10B—C11B	9.7 (3)
C8A—C9A—C10A—C11A	−179.0 (2)	C8B—C9B—C10B—C11B	−168.1 (2)
C15A—C10A—C11A—C12A	1.0 (3)	C15B—C10B—C11B—C12B	0.3 (3)
C9A—C10A—C11A—C12A	179.9 (2)	C9B—C10B—C11B—C12B	179.2 (2)
C10A—C11A—C12A—C13A	−0.9 (4)	C10B—C11B—C12B—C13B	−0.5 (3)
C11A—C12A—C13A—C14A	0.2 (4)	C11B—C12B—C13B—C14B	0.5 (3)
C11A—C12A—C13A—C18A	177.5 (2)	C11B—C12B—C13B—C18B	−179.2 (2)
C12A—C13A—C14A—C15A	0.3 (3)	C12B—C13B—C14B—C15B	−0.3 (4)
C18A—C13A—C14A—C15A	−177.0 (2)	C18B—C13B—C14B—C15B	179.3 (2)
C13A—C14A—C15A—C10A	−0.2 (3)	C13B—C14B—C15B—C10B	0.1 (4)
C11A—C10A—C15A—C14A	−0.5 (3)	C11B—C10B—C15B—C14B	−0.1 (3)
C9A—C10A—C15A—C14A	−179.3 (2)	C9B—C10B—C15B—C14B	−179.1 (2)

N2A—N1A—C16A—O1A	−177.6 (2)	N2B—N1B—C16B—O1B	179.2 (2)
C7A—N1A—C16A—O1A	−1.6 (3)	C7B—N1B—C16B—O1B	1.6 (3)
N2A—N1A—C16A—C17A	0.9 (3)	N2B—N1B—C16B—C17B	−0.4 (3)
C7A—N1A—C16A—C17A	176.8 (2)	C7B—N1B—C16B—C17B	−178.1 (2)

Hydrogen-bond geometry (Å, º)

Cg3 and Cg6 are the centroids of rings C10*A*–C15*A* and C10*B*–C15*B*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8*A*—H8*AB*···O1*B*^{i}	0.99	2.48	3.362 (3)	149
C11*B*—H11*B*···O1*A*^{ii}	0.95	2.56	3.458 (3)	159
C8*B*—H8*BA*···O1*A*	0.99	2.42	3.319 (3)	151
C3*A*—H3*AA*···*Cg*6^{iii}	0.95	2.69	3.550 (3)	151
C3*B*—H3*BA*···*Cg*3^{iv}	0.95	2.95	3.616 (3)	128

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) −*x*, −*y*, −*z*+1; (iii) −*x*+1, −*y*, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1.