Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

6-(2-Benzofuryl)-2-chloro-9-[(4-methoxyphenyl)methyl]-9*H*-purine

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Received 7 May 2007; accepted 8 May 2007

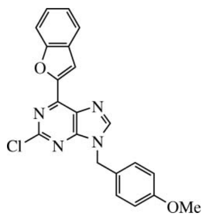
Key indicators: single-crystal X-ray study; *T* = 112 K; mean σ(C–C) = 0.002 Å; *R* factor = 0.036; *wR* factor = 0.094; data-to-parameter ratio = 17.0.

The title compound, $C_{21}H_{15}ClN_4O_2$, is a close analogue of one of the most potent antimycobacterial purines, namely 2-chloro-6-(2-furyl)-9-[(4-methoxyphenyl)methyl]-9*H*-purine. Dimers are stabilized by π–π stacking and C—H$\cdots\pi$ interactions. Intermolecular C—H$\cdots$O hydrogen bonding between the CH group of the purine ring and the O atom in the benzofuran ring, and also π–π stacking in another direction, that result in an average interplanar distance of 3.339 Å between the pyrimidine ring (or 3.424 Å with imidazole ring) and the benzene ring in the benzofuryl group, and 3.318 Å between the furyl ring and the imidazole ring, building a three-dimensional supramolecular network.

Related literature

Bond lengths and angles in the title compound, (I), are in good agreement with those found for 6-furyl- and 6-thienyl-9-benzylpurines (Brændvang & Gundersen, 2007*a*; Mazumdar *et al.*, 2001), and also with the recently reported non-purine analogue 4-(2-furyl)-1-[(4-methoxyphenyl)methyl]-1*H*-pyrazolo[3,4–*d*]pyrimidine (Brændvang & Gundersen, 2007*b*). The molecular packing, as well as the orientations of the furyl and benzene rings, very much resemble the recently reported analogue 2-chloro-6-(2-furanyl)-9-[(4-methoxyphenyl)-methyl]-9*H*-purine (Brændvang & Gundersen, 2007*a*).

For related literature, see: Bakkestuen *et al.* (2000, 2005); Brændvang & Gundersen (2005); Gundersen *et al.* (2002); Liebeskind & Wang (1993).



Experimental

Crystal data

$C_{21}H_{15}ClN_4O_2$
M_r = 390.82
Monoclinic, $P2_1/n$
a = 8.0721 (8) Å
b = 28.668 (3) Å
c = 8.3764 (9) Å
β = 114.876 (2)°
V = 1758.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 112 (2) K
0.3 × 0.2 × 0.2 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.642, $T_{\max}$ = 0.952
16890 measured reflections
4334 independent reflections
3366 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 1.03
4334 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.31 e Å^{-3}
$\Delta\rho_{\min}$ = −0.23 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C26—H26$\cdots Cg1^{\rm i}$	0.95	2.85	3.6453 (18)	141
C8—H8$\cdots$O18$^{\rm ii}$	0.95	2.66	3.6034 (17)	172

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x-1, y, z-1$. $Cg1$ is the centroid of the benzene ring C11–C16.

Table 2
A comparison of selected geometric parameters (Å, °) of (I) and molecules A and B in (II).

	(I)	Molecule A in (II)^a	Molecule B in (II)^a
C6—C17	1.4521 (18)	1.4479 (15)	1.4497 (15)
C10—N9	1.4732 (17)	1.4755 (15)	1.4740 (15)
C10—C11	1.5122 (19)	1.5128 (16)	1.5127 (16)
C14—O22—C23	117.51 (11)	118.12 (10)	116.93 (9)
C15—C14—O22—C23	11.5 (2)	11.24 (17)	−2.45 (17)
C4—N9—C10—C11	79.64 (17)	78.72 (15)	−70.99 (15)
N9—C10—C11—C12	−95.59 (16)	−94.59 (14)	91.21 (13)

Note: (*a*) Braendvang & Gundersen (2007*a*).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Version 1.08; Farrugia, 1997) and *POV-RAY for Windows* (Persistence of Vision Pty Ltd, 2004); software used to prepare material for publication: *SHELXL97* and *WinGX* (Farrugia, 1999).

The authors thank Dr Osamu Sekiguchi, Department of Chemistry, University of Oslo, for the single-crystal data collection and initial refinement.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2252).

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supplementary materials

Acta Cryst. (2007). E**63**, o3036-o3037 [**doi:10.1107/S1600536807022647**]

6-(2-Benzofuryl)-2-chloro-9-[(4-methoxyphenyl)methyl]-9*H*-purine

M. Brændvang and **L.-L. Gundersen**

Comment

We have discovered that certain 6-aryl-9-benzylpurines are potent antimycobacterials *in vitro* and may have a potensial as antitubercular drugs (Bakkestuen *et al.*, 2000; Gundersen *et al.*, 2002; Bakkestuen *et al.*, 2005; Braendvang & Gundersen, 2005). The title compound, (I), was synthesized as a close analog of the previously reported antimycobacterial 2-chloro-6-(2-furanyl)-9-[(4-methoxyphenyl)methyl]-9*H*-purine, (II), (Bakkestuen *et al.*, 2005).

The molecular geometries is illustrated in Fig. 1. The selected bond lenghts and angles are listed in Table 1 and compared with the recently reported X-ray structure of compound (II) (Braendvang & Gundersen, 2007*a*). There are only small differences in bond lenghts and angles in these two compounds, specially molecule A in compound (II) resembles the title compound (I) (Table 1). In compound (I) the angle between the mean plane of the purine ring system and the furyl ring C17/O18/C19—C21 is 4.49 (7)°, or 4.82 (5)° if the mean plane of benzofuryl is used. In compound (II) the angles were 2.31 (6)° in molecule A and 2.79 (5)° in molecule B.

The positions of the benzyl groups are only slightly different in compound (I) and (II) as seen from the torsion angles C4—N9—C10—C11 and N9—C10—C11—C12 (Table 1). The benzene ring C11—C16 is inclined at an angle of 70.68 (6)° to the purine ring in compound (I). Previously reported for compound (II) is 73.64 (5)° in molecule A and 77.80 (4)° in molecule B.

Fig. 2 shows the crystal packing of (I) in the unit cell. The conformation adopted by the benzene rings allows for simultaneous C—H···π interactions, and π–π interactions to form dimers of molecules (Fig. 3). The C—H···π interactions occurs between the C26—H26···$Cg1^{i}$ (Table 2) (*Cg*1 is the centroid of the benzene ring C11—C16) [symmetry code: (i) $2 - x$, $1 - y$, $1 - z$]. In these dimers, π–π interactions occurs between the purine ring system and the benzene ring C19/C20/C24—C27 in the benzofuryl group. In this interaction the benzene ring C19/C20/C24—C27 and the pyrimidine ring N1/C2/N3/C4—C6 are slipped by 18.7 ° relative to their ring perpendiculars (the average interplanar distance between the benzene ring in the benzofuryl group and the pyrimidine ring N1/C2/N3/C4—C6 is 3.339 Å), the ring-centroid to ring-centroid distance being 3.5277 (10) Å. The average interplanar distance between the benzene ring in the benzofuryl group and the imidazole ring C4/C5/N7/C8/N9 is 3.424 Å (the two rings are slipped by 22.8° relative to their ring perpendiculars), the ring-centroid to ring-centroid distance being 3.7161 (10) Å.

The crystal packing (Fig. 2) gives further π–π interactions between the imidazole ring (C4A—N9A) and the furyl ring C17/O18/C19—$C21^{iii}$, the ring-centroid to centroid distance is 3.5084 (10) Å [symmetry code: (iii) $1 - x$, $1 - y$, $1 - z$]. In this interaction the average interplanar distance is 3.318 Å and the two rings are slipped by 19.0° relative to their ring perpendiculars.

Finally, the orientation of the furyl group in compound (I) is stabilized by weak C8—H8···$O18^{ii}$ hydrogen bonding, forming infinite chains of molecules (Table 2 and Fig. 3) [symmetry code: (ii) $x - 1$, y, $z - 1$].

The molecular packing of compound (I) in overall is very similar to the previous reported (II) (Braendvang & Gundersen, 2007*a*).

Experimental

The title compound was synthesized by regioselective Stille coupling using benzofur-2-yl stannane as described for compound (II) (Bakkestuen *et al.*, 2005). The benzofur-2-yl stannane used was made by literature procedure (Liebeskind & Wang, 1993). Crystals suitable for X-ray diffraction studies were obtained from a solution of title compound (27 mg) in CH_2Cl_2 (0.8 ml) with a top layer of heptane (0.8 ml).

Refinement

H atoms were positioned geometrically and allowed to ride and rotate (for the CH_3 group) on their carrier atoms, with C—H = 0.95 (aromatic), 0.99 (CH_2) or 0.98 Å (CH_3) and with $U_{iso}(H) = 1.2U_{eq}(C)$ for CH_2 and aromatic, or $1.5U_{eq}(C)$ for CH_3.

Figures

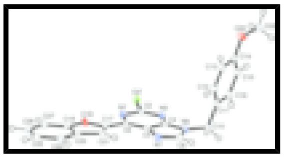


Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

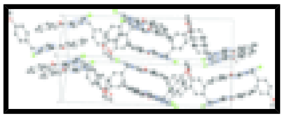


Fig. 2. The packing of (I) in the unit cell. H atoms have been omitted for clarity.

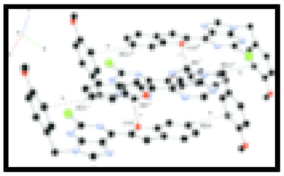


Fig. 3. A partial packing view, showing the intermolecular C—H···π interactions (dashed lines labelled π) between the C26—H26 and the benzyl group (C11—C16) in compound (I). Dashed lines labelled with an asterisk (*) are the intermolecular C8—H8···O18 hydrogen bonding. H atoms not involved in hydrogen-bonding interactions have been omitted for clarity. [symmetry code: (i) $2 - x, 1 - y, 1 - z$; (ii) $x - 1, y, z - 1$; (iii) $1 - x, 1 - y, -z$].

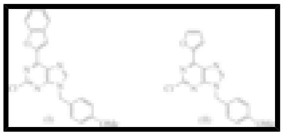


Fig. 4. The structures of (I) and (II).

6-(2-Benzofuryl)-2-chloro-9-[(4-methoxyphenyl)methyl]-9*H*-purine

Crystal data

$C_{21}H_{15}ClN_4O_2$	$F_{000} = 808$
$M_r = 390.82$	$D_x = 1.476$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 7413 reflections
$a = 8.0721 (8)$ Å	$\theta = 2.8–28.9°$
$b = 28.668 (3)$ Å	$\mu = 0.24$ mm^{-1}

c = 8.3764 (9) Å	T = 112 (2) K
β = 114.876 (2)°	Block, colourless
V = 1758.6 (3) Å^3	0.3 × 0.2 × 0.2 mm
Z = 4	

Data collection

Siemens SMART CCD diffractometer	$R_{\rm int}$ = 0.044
Sets of exposures each taken over 0.3° ω rotation scans	$\theta_{\rm max}$ = 29.1°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\rm min}$ = 1.4°
$T_{\rm min}$ = 0.642, $T_{\rm max}$ = 0.952	h = −10→10
16890 measured reflections	k = −38→39
4334 independent reflections	l = −10→11
3366 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2 + 0.2117P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.036	$(\Delta/\sigma)_{\rm max}$ = 0.001
$wR(F^2)$ = 0.094	$\Delta\rho_{\rm max}$ = 0.31 e Å^{-3}
S = 1.03	$\Delta\rho_{\rm min}$ = −0.23 e Å^{-3}
4334 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
255 parameters	Extinction coefficient: 0.0045 (10)

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.

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

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
C23	0.4460 (2)	0.75117 (6)	−0.4061 (2)	0.0304 (3)
H23C	0.4944	0.7779	−0.4457	0.046*
H23B	0.3129	0.7501	−0.4719	0.046*
H23A	0.4994	0.7224	−0.4266	0.046*
C14	0.42248 (18)	0.72315 (5)	−0.14688 (19)	0.0219 (3)
C15	0.33819 (19)	0.68194 (5)	−0.22890 (18)	0.0220 (3)
H15	0.326	0.6747	−0.344	0.026*
C16	0.27211 (19)	0.65160 (5)	−0.14000 (18)	0.0224 (3)

H16	0.213	0.6237	−0.1964	0.027*
C11	0.29012 (18)	0.66101 (5)	0.02899 (18)	0.0206 (3)
C12	0.3764 (2)	0.70225 (5)	0.1092 (2)	0.0256 (3)
H12	0.3907	0.7092	0.2251	0.031*
C13	0.4416 (2)	0.73323 (5)	0.0223 (2)	0.0270 (3)
H13	0.4993	0.7613	0.0782	0.032*
C10	0.21757 (19)	0.62721 (5)	0.1228 (2)	0.0251 (3)
H10B	0.1899	0.6444	0.2111	0.03*
H10A	0.1022	0.6134	0.0364	0.03*
C8	0.3488 (2)	0.54524 (5)	0.14963 (19)	0.0248 (3)
H8	0.2588	0.5346	0.04	0.03*
C5	0.58017 (18)	0.54779 (4)	0.39524 (17)	0.0190 (3)
C6	0.73824 (18)	0.54209 (4)	0.55173 (17)	0.0182 (3)
C2	0.70456 (19)	0.61808 (5)	0.61788 (18)	0.0198 (3)
C4	0.49637 (18)	0.59170 (5)	0.36956 (18)	0.0192 (3)
C17	0.84136 (18)	0.49884 (4)	0.59799 (18)	0.0185 (3)
C21	0.82115 (18)	0.45845 (4)	0.50752 (18)	0.0201 (3)
H21	0.7293	0.4516	0.3937	0.024*
C20	0.96580 (18)	0.42808 (5)	0.61741 (18)	0.0192 (3)
C24	1.02383 (19)	0.38258 (5)	0.60394 (19)	0.0223 (3)
H24	0.9607	0.3644	0.5013	0.027*
C25	1.1748 (2)	0.36497 (5)	0.74343 (19)	0.0240 (3)
H25	1.2162	0.3344	0.7357	0.029*
C26	1.2679 (2)	0.39127 (5)	0.8958 (2)	0.0246 (3)
H26	1.3708	0.378	0.9897	0.03*
C27	1.2137 (2)	0.43633 (5)	0.91346 (19)	0.0244 (3)
H27	1.2763	0.4543	1.0168	0.029*
C19	1.06353 (18)	0.45333 (4)	0.77165 (18)	0.0199 (3)
N9	0.34760 (15)	0.58943 (4)	0.21140 (15)	0.0211 (3)
N7	0.48406 (16)	0.51863 (4)	0.25380 (15)	0.0235 (3)
N1	0.80044 (15)	0.57858 (4)	0.66414 (15)	0.0194 (2)
N3	0.55232 (16)	0.62840 (4)	0.47883 (15)	0.0204 (2)
O22	0.49164 (14)	0.75576 (3)	−0.22214 (14)	0.0290 (2)
O18	0.98871 (13)	0.49710 (3)	0.76115 (12)	0.0209 (2)
Cl2	0.79826 (5)	0.664269 (11)	0.76375 (5)	0.02636 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C23	0.0249 (8)	0.0330 (8)	0.0319 (8)	0.0020 (6)	0.0106 (7)	0.0137 (7)
C14	0.0175 (7)	0.0184 (6)	0.0280 (7)	0.0015 (5)	0.0078 (6)	0.0063 (5)
C15	0.0217 (7)	0.0208 (7)	0.0216 (7)	0.0009 (5)	0.0071 (6)	0.0026 (5)
C16	0.0201 (7)	0.0171 (6)	0.0253 (7)	−0.0006 (5)	0.0049 (6)	0.0029 (5)
C11	0.0151 (6)	0.0217 (7)	0.0230 (7)	0.0038 (5)	0.0061 (5)	0.0069 (5)
C12	0.0252 (8)	0.0272 (7)	0.0242 (7)	0.0012 (6)	0.0101 (6)	−0.0005 (6)
C13	0.0277 (8)	0.0196 (7)	0.0313 (8)	−0.0036 (6)	0.0100 (7)	−0.0031 (6)
C10	0.0174 (7)	0.0273 (7)	0.0278 (8)	0.0036 (6)	0.0066 (6)	0.0109 (6)
C8	0.0247 (7)	0.0228 (7)	0.0230 (7)	−0.0054 (6)	0.0063 (6)	0.0021 (5)

C5	0.0196 (7)	0.0170 (6)	0.0214 (7)	−0.0017 (5)	0.0096 (6)	0.0031 (5)
C6	0.0185 (7)	0.0173 (6)	0.0202 (7)	−0.0005 (5)	0.0094 (6)	0.0027 (5)
C2	0.0209 (7)	0.0185 (6)	0.0215 (7)	0.0005 (5)	0.0104 (6)	0.0011 (5)
C4	0.0169 (6)	0.0203 (6)	0.0211 (7)	0.0002 (5)	0.0087 (6)	0.0052 (5)
C17	0.0170 (6)	0.0186 (6)	0.0192 (7)	−0.0011 (5)	0.0069 (5)	0.0032 (5)
C21	0.0194 (7)	0.0194 (6)	0.0203 (7)	−0.0012 (5)	0.0072 (6)	0.0017 (5)
C20	0.0192 (7)	0.0172 (6)	0.0224 (7)	−0.0013 (5)	0.0099 (6)	0.0017 (5)
C24	0.0234 (7)	0.0181 (6)	0.0276 (7)	−0.0025 (5)	0.0128 (6)	−0.0012 (5)
C25	0.0255 (8)	0.0163 (6)	0.0352 (8)	0.0025 (5)	0.0178 (7)	0.0039 (6)
C26	0.0213 (7)	0.0236 (7)	0.0287 (8)	0.0047 (5)	0.0103 (6)	0.0079 (6)
C27	0.0248 (7)	0.0218 (7)	0.0239 (7)	0.0011 (6)	0.0077 (6)	0.0015 (6)
C19	0.0216 (7)	0.0153 (6)	0.0253 (7)	0.0010 (5)	0.0123 (6)	0.0029 (5)
N9	0.0184 (6)	0.0206 (6)	0.0218 (6)	−0.0006 (4)	0.0061 (5)	0.0051 (4)
N7	0.0238 (6)	0.0197 (6)	0.0230 (6)	−0.0033 (5)	0.0058 (5)	0.0020 (5)
N1	0.0200 (6)	0.0178 (5)	0.0215 (6)	0.0013 (4)	0.0097 (5)	0.0019 (4)
N3	0.0204 (6)	0.0189 (6)	0.0224 (6)	0.0015 (4)	0.0094 (5)	0.0026 (4)
O22	0.0292 (6)	0.0234 (5)	0.0328 (6)	−0.0054 (4)	0.0115 (5)	0.0074 (4)
O18	0.0216 (5)	0.0161 (5)	0.0214 (5)	0.0033 (4)	0.0053 (4)	0.0015 (4)
Cl2	0.0269 (2)	0.01996 (17)	0.02673 (19)	0.00263 (13)	0.00591 (15)	−0.00372 (13)

Geometric parameters (Å, °)

C23—O22	1.4318 (19)	C5—C6	1.4022 (19)
C23—H23C	0.98	C6—N1	1.3548 (17)
C23—H23B	0.98	C6—C17	1.4521 (18)
C23—H23A	0.98	C2—N3	1.3229 (18)
C14—O22	1.3708 (16)	C2—N1	1.3338 (17)
C14—C13	1.390 (2)	C2—Cl2	1.7439 (14)
C14—C15	1.3918 (19)	C4—N3	1.3420 (17)
C15—C16	1.3892 (19)	C4—N9	1.3650 (18)
C15—H15	0.95	C17—C21	1.3556 (19)
C16—C11	1.387 (2)	C17—O18	1.3847 (16)
C16—H16	0.95	C21—C20	1.4368 (18)
C11—C12	1.393 (2)	C21—H21	0.95
C11—C10	1.5122 (19)	C20—C19	1.3994 (19)
C12—C13	1.385 (2)	C20—C24	1.4064 (19)
C12—H12	0.95	C24—C25	1.381 (2)
C13—H13	0.95	C24—H24	0.95
C10—N9	1.4732 (17)	C25—C26	1.398 (2)
C10—H10B	0.99	C25—H25	0.95
C10—H10A	0.99	C26—C27	1.3914 (19)
C8—N7	1.3169 (18)	C26—H26	0.95
C8—N9	1.3699 (18)	C27—C19	1.3810 (19)
C8—H8	0.95	C27—H27	0.95
C5—N7	1.3896 (18)	C19—O18	1.3790 (15)
C5—C4	1.4021 (18)		
O22—C23—H23C	109.5	N3—C2—N1	131.02 (13)
O22—C23—H23B	109.5	N3—C2—Cl2	114.55 (10)
H23C—C23—H23B	109.5	N1—C2—Cl2	114.42 (10)

O22—C23—H23A	109.5	N3—C4—N9	127.27 (12)
H23C—C23—H23A	109.5	N3—C4—C5	126.66 (12)
H23B—C23—H23A	109.5	N9—C4—C5	106.07 (12)
O22—C14—C13	115.79 (12)	C21—C17—O18	111.86 (11)
O22—C14—C15	124.13 (13)	C21—C17—C6	131.26 (13)
C13—C14—C15	120.09 (13)	O18—C17—C6	116.88 (11)
C16—C15—C14	119.02 (13)	C17—C21—C20	106.57 (12)
C16—C15—H15	120.5	C17—C21—H21	126.7
C14—C15—H15	120.5	C20—C21—H21	126.7
C11—C16—C15	121.73 (13)	C19—C20—C24	118.46 (12)
C11—C16—H16	119.1	C19—C20—C21	105.57 (11)
C15—C16—H16	119.1	C24—C20—C21	135.97 (13)
C16—C11—C12	118.28 (13)	C25—C24—C20	118.44 (13)
C16—C11—C10	120.54 (13)	C25—C24—H24	120.8
C12—C11—C10	121.17 (13)	C20—C24—H24	120.8
C13—C12—C11	120.94 (14)	C24—C25—C26	121.29 (13)
C13—C12—H12	119.5	C24—C25—H25	119.4
C11—C12—H12	119.5	C26—C25—H25	119.4
C12—C13—C14	119.92 (13)	C27—C26—C25	121.69 (13)
C12—C13—H13	120	C27—C26—H26	119.2
C14—C13—H13	120	C25—C26—H26	119.2
N9—C10—C11	112.54 (11)	C19—C27—C26	115.96 (13)
N9—C10—H10B	109.1	C19—C27—H27	122
C11—C10—H10B	109.1	C26—C27—H27	122
N9—C10—H10A	109.1	O18—C19—C27	125.35 (12)
C11—C10—H10A	109.1	O18—C19—C20	110.50 (11)
H10B—C10—H10A	107.8	C27—C19—C20	124.15 (12)
N7—C8—N9	114.90 (13)	C4—N9—C8	105.52 (11)
N7—C8—H8	122.6	C4—N9—C10	127.12 (12)
N9—C8—H8	122.6	C8—N9—C10	127.32 (12)
N7—C5—C4	110.43 (12)	C8—N7—C5	103.09 (11)
N7—C5—C6	133.55 (12)	C2—N1—C6	116.97 (12)
C4—C5—C6	116.02 (12)	C2—N3—C4	110.28 (11)
N1—C6—C5	119.02 (12)	C14—O22—C23	117.51 (11)
N1—C6—C17	118.07 (12)	C19—O18—C17	105.49 (10)
C5—C6—C17	122.90 (12)		

O22—C14—C15—C16	−179.57 (13)	C25—C26—C27—C19	−0.2 (2)
C13—C14—C15—C16	0.7 (2)	C26—C27—C19—O18	−179.33 (13)
C14—C15—C16—C11	−0.9 (2)	C26—C27—C19—C20	0.7 (2)
C15—C16—C11—C12	0.3 (2)	C24—C20—C19—O18	179.47 (12)
C15—C16—C11—C10	−179.72 (13)	C21—C20—C19—O18	−0.71 (15)
C16—C11—C12—C13	0.4 (2)	C24—C20—C19—C27	−0.5 (2)
C10—C11—C12—C13	−179.60 (13)	C21—C20—C19—C27	179.31 (13)
C11—C12—C13—C14	−0.5 (2)	N3—C4—N9—C8	179.55 (13)
O22—C14—C13—C12	−179.79 (13)	C5—C4—N9—C8	−0.27 (14)
C15—C14—C13—C12	−0.1 (2)	N3—C4—N9—C10	1.8 (2)
C16—C11—C10—N9	84.43 (16)	C5—C4—N9—C10	−178.07 (12)
C12—C11—C10—N9	−95.59 (16)	N7—C8—N9—C4	0.36 (16)
N7—C5—C6—N1	178.71 (13)	N7—C8—N9—C10	178.16 (12)

C4—C5—C6—N1	−1.07 (18)	C11—C10—N9—C4	79.64 (17)
N7—C5—C6—C17	−0.1 (2)	C11—C10—N9—C8	−97.70 (16)
C4—C5—C6—C17	−179.86 (12)	N9—C8—N7—C5	−0.28 (16)
N7—C5—C4—N3	−179.71 (12)	C4—C5—N7—C8	0.10 (15)
C6—C5—C4—N3	0.1 (2)	C6—C5—N7—C8	−179.70 (14)
N7—C5—C4—N9	0.11 (15)	N3—C2—N1—C6	1.5 (2)
C6—C5—C4—N9	179.95 (11)	Cl2—C2—N1—C6	−177.23 (9)
N1—C6—C17—C21	−174.32 (14)	C5—C6—N1—C2	0.43 (18)
C5—C6—C17—C21	4.5 (2)	C17—C6—N1—C2	179.28 (12)
N1—C6—C17—O18	4.85 (17)	N1—C2—N3—C4	−2.3 (2)
C5—C6—C17—O18	−176.35 (11)	Cl2—C2—N3—C4	176.42 (9)
O18—C17—C21—C20	−0.57 (15)	N9—C4—N3—C2	−178.44 (13)
C6—C17—C21—C20	178.64 (13)	C5—C4—N3—C2	1.34 (19)
C17—C21—C20—C19	0.76 (15)	C13—C14—O22—C23	−168.83 (13)
C17—C21—C20—C24	−179.47 (15)	C15—C14—O22—C23	11.5 (2)
C19—C20—C24—C25	−0.12 (19)	C27—C19—O18—C17	−179.64 (13)
C21—C20—C24—C25	−179.87 (14)	C20—C19—O18—C17	0.38 (14)
C20—C24—C25—C26	0.6 (2)	C21—C17—O18—C19	0.13 (14)
C24—C25—C26—C27	−0.4 (2)	C6—C17—O18—C19	−179.20 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C26—H26···Cg1^{i}	0.95	2.85	3.6453 (18)	141
C8—H8···O18^{ii}	0.95	2.66	3.6034 (17)	172

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) *x*−1, *y*, *z*−1.

Table 1. A comparison of selected geometric parameters (Å, °) of (I) and molecules A and B in (II)

	Compound (I)	Molecule A in (II)^{a}	Molecule B in (II)^{a}
C6—C17	1.4521 (18)	1.4479 (15)	1.4497 (15)
C10—N9	1.4732 (17)	1.4755 (15)	1.4740 (15)
C10—C11	1.5122 (19)	1.5128 (16)	1.5127 (16)
C14—O22—C23	117.51 (11)	118.12 (10)	116.93 (9)
C15—C14—O22—C23	11.5 (2)	11.24 (17)	-2.45 (17)
C4—N9—C10—C11	79.64 (17)	78.72 (15)	-70.99 (15)
N9—C10—C11—C12	-95.59 (16)	-94.59 (14)	91.21 (13)

Notes: (*a*) Braendvang & Gundersen (2007*a*).

Fig. 1

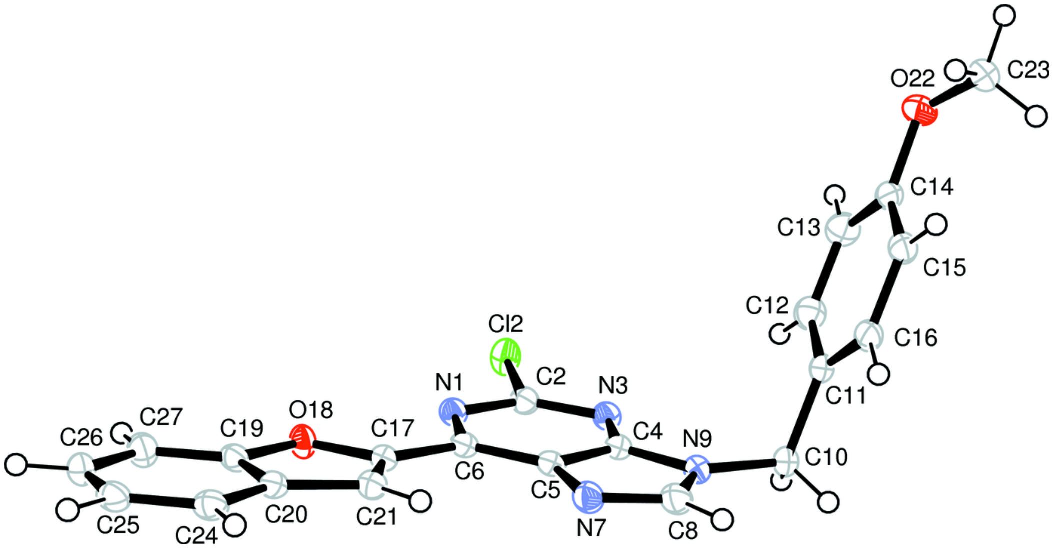

O22
C23
C14
C13
C15
C12
C16
Cl2
C11
C2
N1
N3
O18
C17
C4
N9
C27
C19
C26
C10
C6
C5
C21
C20
C8
C25
N7
C24

Fig. 2

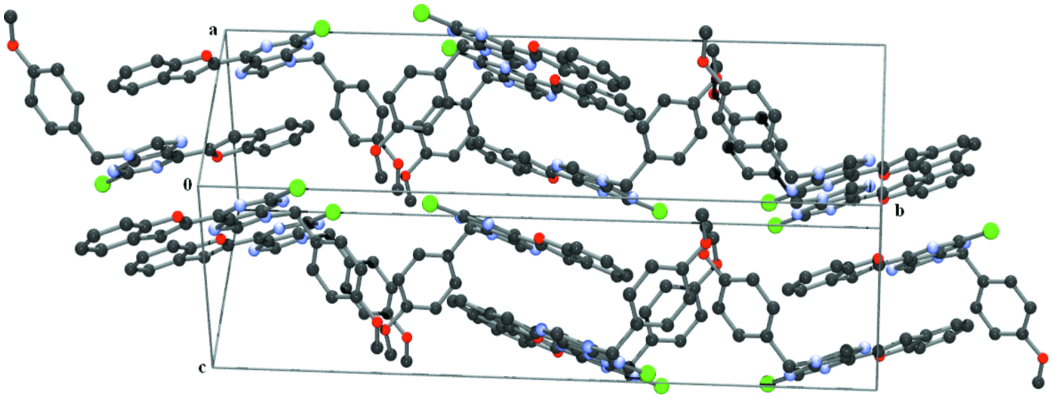


Fig. 3

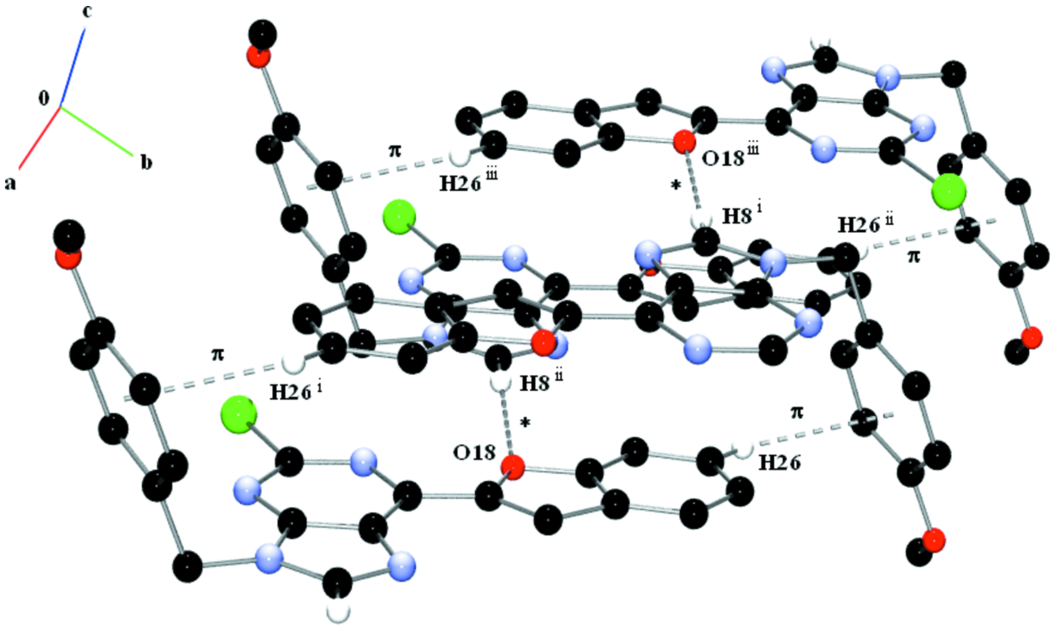
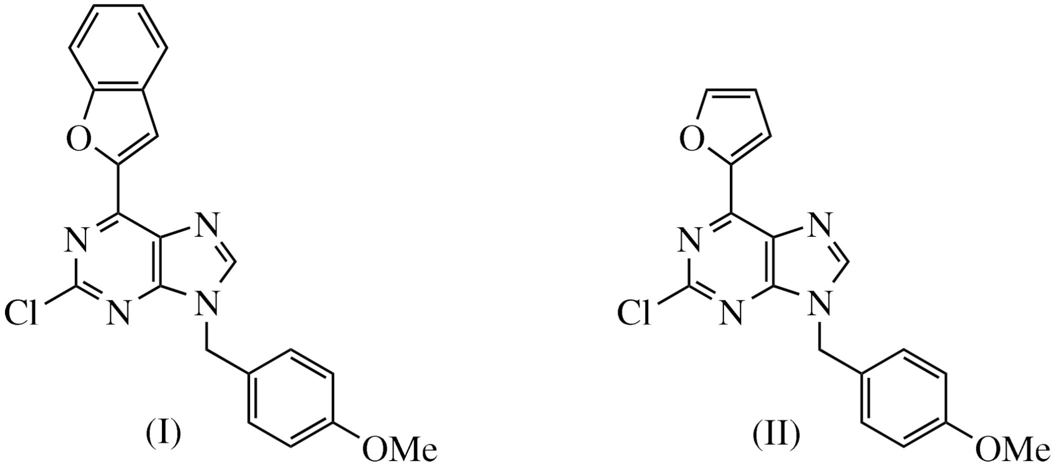

c
0
a
b
π
$\mathrm{H26}^{iii}$
$\mathrm{O18}^{iii}$
*
$\mathrm{H8}^{i}$
$\mathrm{H26}^{ii}$
π
π
$\mathrm{H26}^{i}$
$\mathrm{H8}^{ii}$
*
O18
π
H26

Fig. 4



(I)

(II)