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Halogenated *C*,*N*-diarylacetamides: molecular conformations and supramolecular assembly

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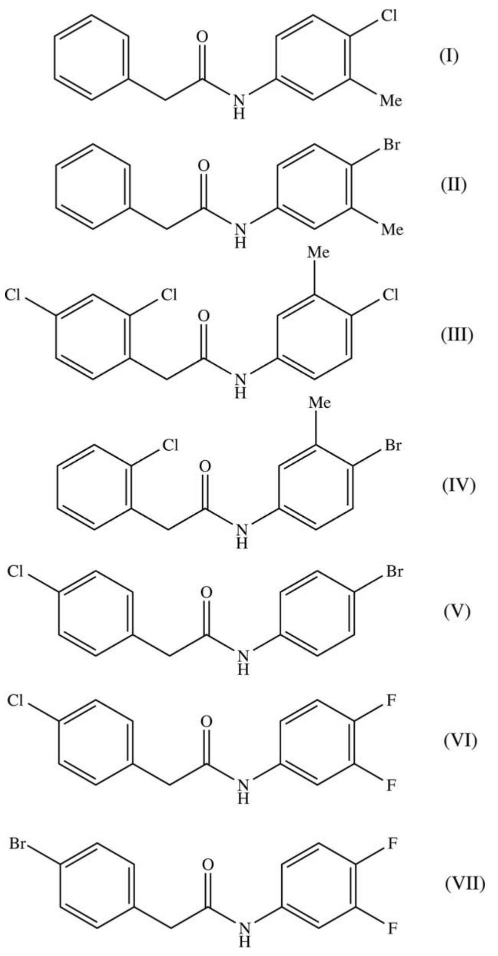
The structures of four halogenated *N*,2-diarylacetamides are reported and compared with a range of analogues. *N*-(4-Chloro-3-methylphenyl)-2-phenylacetamide, $C_{15}H_{14}ClNO$, (I), and *N*-(4-bromo-3-methylphenyl)-2-phenylacetamide, $C_{15}H_{14}BrNO$, (II), are isostructural in the space group $P\bar{1}$. The molecules of (I) and (II) are linked into chains of rings by a combination of N—H$\cdots$O and C—H$\cdots\pi$(arene) hydrogen bonds. The molecules of *N*-(4-chloro-3-methylphenyl)-2-(2,4-dichlorophenyl)acetamide, $C_{15}H_{12}Cl_3NO$, (III), and *N*-(4-bromo-3-methylphenyl)-2-(2-chlorophenyl)acetamide, $C_{15}H_{13}BrClNO$, (IV), are linked into simple *C*(4) chains by N—H$\cdots$O hydrogen bonds, but significant C—H$\cdots\pi$(arene) interactions are absent. The *N*-aryl groups in compounds (III) and (IV) adopt a different orientation, by *ca* 180°, from that of the corresponding groups in compounds (I) and (II), but otherwise the conformations of (I)–(IV) are very similar. Comparisons are drawn between compounds (I) and (IV) and a range of analogues of the type $R^1CH_2CONHR^2$, where R^2 represents a halogenated aryl ring and R^1 represents either another halogenated aryl ring or a naphthalen-1-yl unit.

Keywords: crystal structure; acetamides; *C*,*N*-diarylacetamides; molecular conformation; supramolecular assembly; hydrogen bonding; benzyl penicillins.

1. Introduction

Substituted acetamides of the type $R^1CH_2CONHR^2$, where R^1 and R^2 are aromatic substituents, are of interest as they have some resemblance to benzyl penicillins (Pitt, 1952; Csöregh & Palm, 1977; Kojić-Prodić & Ružoć-Toroš, 1978; Mijin & Marinkovic, 2006; Mijin *et al.*, 2008). We report here the molecular structures and supramolecular assembly of four closely related amides, namely *N*-(4-chloro-3-methylphenyl)-2-phenylacetamide, (I), *N*-(4-bromo-3-methylphenyl)-2-phenylacetamide, (II), *N*-(4-chloro-3-methylphenyl)-2-(2,4-dichlorophenyl)acetamide, (III), and *N*-(4-bromo-3-methylphenyl)-2-(2-chlorophenyl)acetamide, (IV) (see Scheme 1).



Scheme 1

The purposes of this study are: (i) the comparison of the molecular conformations and the supramolecular assembly across a series of amides of the type $R^1CH_2CONHR^2$, where R^1 and R^2 represent either phenyl (in the case of R^1) or halogeno-substituted phenyl groups (for both R^1 and R^2), including not only compounds (I)–(IV), but also their recently reported analogues (V)–(VII) (see Scheme 1); (ii) the extension of this comparison of supramolecular assembly patterns to include analogues where R^1 represents the naphthalen-1-yl unit, (VIII)–(XI) (see Scheme 2), where there is greater scope for the occurrence of π–π stacking interactions. Compounds (V)–(XI) have all been the subjects of individual structure reports, some of them quite brief, and no comparisons between them have been drawn. Accordingly, it is worthwhile to draw together these disparate structural reports for the purposes of comparison, and this we undertake here. We also briefly consider the effects on the supramolecular assembly when R^2 represents an N-heterocyclic group, thereby intro-

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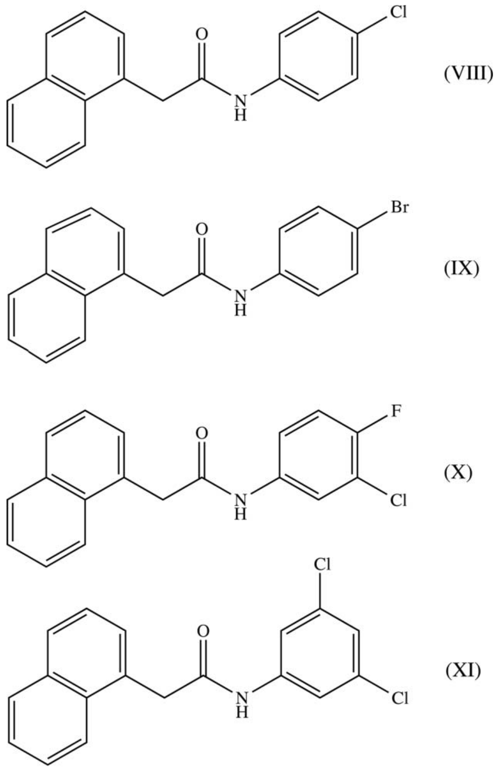
ducing into the molecular constitution one or more further potential hydrogen-bond acceptors. Compounds (I)–(IV) were all prepared by a condensation reaction between a substituted aniline and either phenylacetic acid, for compounds (I) and (II), or a substituted phenylacetic acid, for compounds (III) and (IV), using a tenfold molar excess of 3-[3-(dimethylamino)propyl]-1-ethylcarbodiimide hydrochloride as the amide coupling agent.



Scheme 2

2. Experimental

2.1. Synthesis and crystallization

For the synthesis of compounds (I)–(IV), a mixture of 1 mmol each of the appropriately substituted phenylacetic acid and aniline precursors was dissolved in dichloromethane (20 ml) in the presence of 3-[3-(dimethylamino)propyl]-1-ethylcarbodiimide hydrochloride (1.0 g, 10 mmol) and triethylamine (2 mmol). The mixtures were stirred at 273 K for 3 h, and then each was poured with stirring into an ice-cold aqueous hydrogen chloride solution (100 ml of 10% solution). The resulting mixtures were extracted with dichloromethane (3 × 20 ml); each of the combined organic extracts was then washed with an excess of aqueous sodium hydrogen carbonate solution and with brine, after which the solvent was removed under reduced pressure. Slow evaporation, at ambient temperature and in the presence of air, of solutions in methanol gave colourless crystals of compounds (I)–(IV) suitable for single-crystal X-ray diffraction. Compound (I): yield 77%, m.p. 397–399 K; analysis found: C 69.3, H 5.5, N 5.4%; $C_{15}H_{14}ClNO$ requires: C 69.4, H 5.4, N 5.4%. Compound (II): yield 78%, m.p. 407–409 K; analysis found: C 59.2, H 4.7, N 4.6%; $C_{15}H_{14}BrNO$ requires: C 59.2, H 4.6, N 4.6%. Compound (III): yield 80%, m.p. 457–459 K; analysis found: C 54.8, H 3.7, N 4.2%; $C_{15}H_{12}Cl_3NO$ requires: C 54.8, H 3.7, N 4.3%. Compound (IV): yield 83%, m.p. 454–456 K; analysis found: C 53.2, H 3.9, N 4.2%; $C_{15}H_{13}BrClNO$ requires: C 53.2, H 3.9, N 4.1%.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All H atoms were located in difference maps and then treated as riding atoms, with C—H = 0.95 (aromatic), 0.98 (CH_3) or 0.99 Å (CH_2) and N—H = 0.88 Å, and with $U_{\rm iso}({\rm H}) = kU_{\rm eq}({\rm N,O})$, where k = 1.5 for the methyl groups, which were permitted to rotate but not to tilt, and 1.2 for all other H atoms. For compound (IV), the low-angle reflection 200, which had been attenuated by the beam stop, was omitted from the final refinement. The absolute configuration of (III) in the crystal selected for data collection was established by means of the Flack x parameter (Flack, 1983), x = 0.02 (4), calculated by the use of 697 quotients $[(I+)-(I-)]/[(I+)+(I-)]$ (Parsons *et al.*, 2013).

3. Results and discussion

Compounds (I) (Fig. 1) and (II) (Fig. 2) are isostructural in the space group $P\overline{1}$, while compounds (III) (Fig. 3) and (IV) (Fig. 4) both crystallize in monoclinic space groups, *viz.* $P2_1$ and $P2_1/c$ respectively. Compound (V) also crystallizes in $P2_1/c$ (Fun, Shahani *et al.*, 2012), while compounds (VI) (Praveen *et al.*, 2013*b*) and (VII) (Praveen *et al.*, 2013*a*) are isostructural in the space group $P2_12_12_1$, although neither of

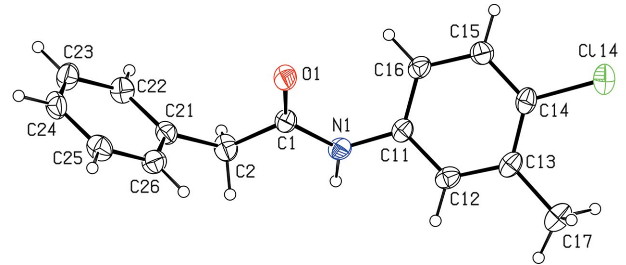


Figure 1
The molecular structure of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

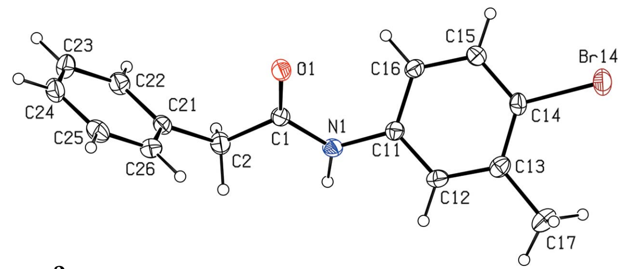


Figure 2
The molecular structure of compound (II), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

Table 1
Experimental details.

	(I)	(II)	(III)	(IV)
Crystal data				
Chemical formula	$C_{15}H_{14}ClNO$	$C_{15}H_{14}BrNO$	$C_{15}H_{12}Cl_3NO$	$C_{15}H_{13}BrClNO$
M_r	259.72	304.18	328.61	338.62
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$	Monoclinic, $P2_1$	Monoclinic, $P2_1/c$
Temperature (K)	173	173	173	173
a, b, c (Å)	5.0039 (7), 10.7525 (12), 12.6177 (12)	4.9995 (3), 10.8392 (4), 12.7301 (7)	11.8441 (7), 4.7288 (3), 13.0981 (7)	11.8458 (8), 4.7282 (3), 25.0757 (15)
α, β, γ (°)	108.615 (10), 91.771 (11), 90.167 (11)	108.149 (4), 91.968 (5), 90.310 (4)	90, 101.310 (6), 90	90, 98.133 (5), 90
V (Å^3)	643.01 (14)	655.05 (6)	719.36 (7)	1390.35 (15)
Z	2	2	2	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	2.51	4.16	5.71	3.14
Crystal size (mm)	0.28 × 0.16 × 0.08	0.32 × 0.18 × 0.08	0.16 × 0.08 × 0.06	0.38 × 0.12 × 0.08
Data collection				
Diffractometer	Agilent Eos Gemini diffractometer	Agilent Eos Gemini diffractometer	Agilent Eos Gemini diffractometer	Agilent Eos Gemini diffractometer
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2012)	Multi-scan (*CrysAlis PRO*; Agilent, 2012)	Multi-scan (*CrysAlis PRO*; Agilent, 2012)	Multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min}, T_{max}	0.413, 0.818	0.286, 0.818	0.256, 0.710	0.373, 0.778
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3772, 2447, 1865	3876, 2515, 2276	4196, 2566, 2214	10821, 3201, 2177
R_{int}	0.032	0.039	0.039	0.084
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.618	0.618	0.617	0.651
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.187, 1.09	0.042, 0.110, 1.07	0.058, 0.155, 1.07	0.064, 0.141, 1.08
No. of reflections	2447	2515	2566	3201
No. of parameters	164	164	182	173
No. of restraints	0	0	1	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.30	0.72, −0.45	0.55, −0.29	0.58, −0.67
Absolute structure	–	–	Flack x determined using 697 quotients (Parsons *et al.*, 2013)	–
Absolute structure parameter	–	–	−0.02 (4)	–

Computer programs: *CrysAlis PRO* (Agilent, 2012), *CrysAlis RED* (Agilent, 2012), *SUPERFLIP* (Palatinus & Chapuis, 2007), *SHELXL2014* (Sheldrick, 2008, 2014) and *PLATON* (Spek, 2009).

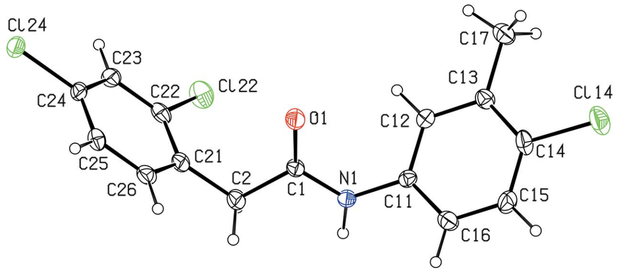


Figure 3
The molecular structure of compound (III), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

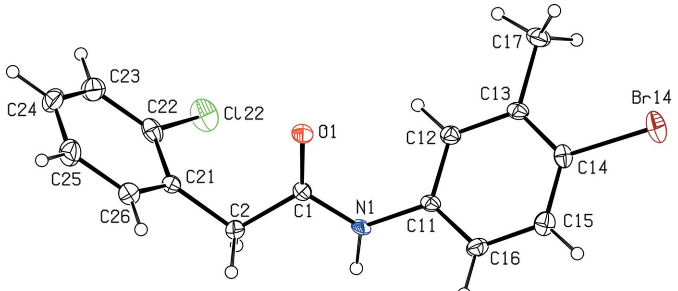


Figure 4
The molecular structure of compound (IV), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

the original structure reports on (VI) and (VII) mentioned the other.

The 4-halogeno-3-methylphenyl units in compounds (III) and (IV) adopt a different orientation from those in compounds (I) and (II), corresponding to a rotation of approximately 180° around the N1—C11 bond (*cf.* Figs. 1–4). Apart from this difference, however, the molecular conformations of compounds (I)–(VII) are all very similar, as demonstrated by the torsion angles (Table 2) which define the

Table 2
Selected torsion and dihedral angles (°) for compounds (I)–(VII).

Compound	θ_1	θ_2	θ_3	θ_4	θ_5
(I)	175.8 (3)	144.4 (3)	161.6 (3)	109.2 (4)	71.96 (16)
(II)	175.6 (1)	144.2 (3)	159.1 (2)	110.5 (3)	72.03 (14)
(III)	−177.5 (5)	134.5 (7)	−177.8 (6)	79.3 (8)	63.5 (3)
(IV)	−177.0 (4)	131.9 (4)	−173.8 (4)	75.5 (5)	60.1 (2)
(V)	−177.6 (4)	133.5 (4)	174.7 (4)	89.9 (5)	68.21 (19)
(VI)	−173.4 (3)	139.2 (4)	−175.1 (3)	80.6 (4)	65.21 (18)
(VII)	−173.6 (5)	138.7 (6)	−175.4 (5)	83.5 (7)	66.4 (3)

Notes: θ_1 represents the torsion angle C2—C1—N1—C11; θ_2 represents the torsion angle C1—N1—C11—C12 for compounds (I) and (II), and the torsion angle C1—N1—C11—C16 for compounds (III) and (IV); θ_3 represents the torsion angle N1—C1—C2—C21; θ_4 represents the torsion angle C1—C2—C21—C22; θ_5 represents the dihedral angle between the two ring planes. For compounds (V)–(VII), the original atom numbering has been modified to match that in compound (I).

Table 3
Hydrogen bonds and short intermolecular contacts (Å, °) for compounds (I)–(IV).

*Cg*1 represents the centroid of the C21–C26 ring.

Compound	$D-\mathrm{H}\cdots A$	$D-\mathrm{H}$	$\mathrm{H}\cdots A$	$D\cdots A$	$D-\mathrm{H}\cdots A$
(I)	$\mathrm{N1-H1\cdots O1^{i}}$	0.88	2.03	2.878 (3)	161
	$\mathrm{C2-H2}B\cdots Cg1^{\mathrm{i}}$	0.99	2.81	3.546 (4)	132
(II)	$\mathrm{N1-H1\cdots O1^{i}}$	0.88	2.03	2.868 (3)	160
	$\mathrm{C2-H2}B\cdots Cg1^{\mathrm{i}}$	0.99	2.78	3.546 (3)	135
(III)	$\mathrm{N1-H1\cdots O1^{ii}}$	0.88	1.96	2.818 (7)	166
	$\mathrm{C2-H2}A\cdots Cg1^{\mathrm{ii}}$	0.99	2.96	3.498 (8)	115
(IV)	$\mathrm{N1-H1\cdots O1^{ii}}$	0.88	1.93	2.802 (4)	170
	$\mathrm{C2-H2}B\cdots Cg1^{\mathrm{ii}}$	0.99	2.99	3.552 (5)	117

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

orientation of the phenyl and benzyl substituents relative to the central *trans*-planar amide unit. The conformational similarity is confirmed by the narrow range spanned by the dihedral angle between the two aryl rings in each compound, ranging from 60.1 (2)° in compound (IV) to 72.03 (14)° in compound (II). The molecular conformations in (I)–(VII) thus appear to be largely independent of the number, nature and location of the halogeno substituents. The molecules of compounds (I)–(VII) are all conformationally chiral, and the centrosymmetric space groups for compounds (I), (II), (IV) and (V) confirm that equal numbers of the two conformational enantiomers are present in each case. For compounds (III), (VI) and (VII), on the other hand, which all crystallize in Sohncke space groups, only one conformational enantiomer is present in each crystal, provided that these crystals are untwinned, which appears to be the case for all of them. For each of these compounds, the absolute configuration of the molecules in the crystal selected for data collection was established by means of the Flack *x* parameter (Flack, 1983; Parsons *et al.*, 2013), but it seems probable that all three crystallize as conformational conglomerates, rather than as conformational racemates, as for compounds (I), (II), (IV) and (V).

In each of the isomorphous compounds (I) and (II), molecules related by translation are linked by $\mathrm{N-H\cdots O}$ hydrogen bonds (Table 3) to form *C*(4) (Bernstein *et al.*, 1995) chains running parallel to the [100] direction. These chains are modestly reinforced by a $\mathrm{C-H}\cdots\pi$(arene) interaction, also involving molecules related by translation, so forming a chain of rings (Fig. 5). Two chains of this type pass through each unit cell, but there are no direction-specific interactions between adjacent chains. The molecules in compounds (III) and (IV) are also linked into *C*(4) chains by $\mathrm{N-H\cdots O}$ hydrogen bonds, in each case running parallel to the [010] direction. Despite the presence of 2_1 screw axes in (III) and (IV), the chains again comprise molecules related by translation. However, the intermolecular $\mathrm{C-H}\cdots\pi$(arene) contacts in (III) and (IV) have rather long $\mathrm{H}\cdots Cg$ distances and small $\mathrm{C-H}\cdots Cg$ angles (Table 3), and they are probably not structurally significant. Hence, the supramolecular assembly in each of (III) and (IV) consists of simple *C*(4) chains (Figs. 6 and 7),

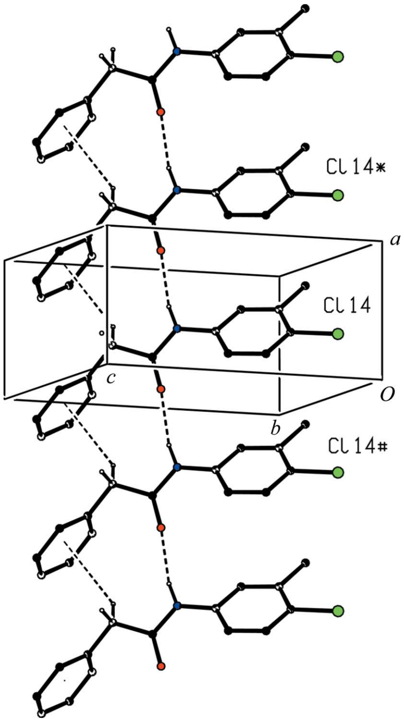


Figure 5
Part of the crystal structure of compound (I), showing the formation of a hydrogen-bonded chain of rings parallel to [100]. Hydrogen bonds are shown as dashed lines and, for the sake of clarity, H atoms bonded to C atoms other than C2 have been omitted. Cl atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions ($x + 1, y, z$) and ($x - 1, y, z$), respectively.

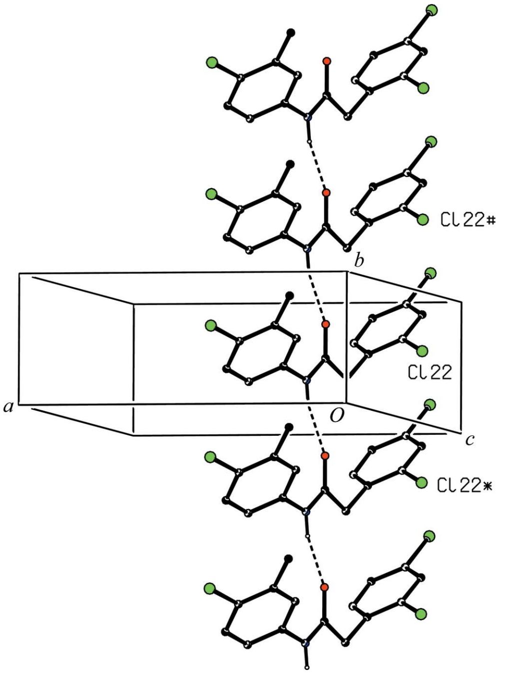


Figure 6
Part of the crystal structure of compound (III), showing the formation of a *C*(4) hydrogen-bonded chain parallel to [010]. Hydrogen bonds are shown as dashed lines and, for the sake of clarity, H atoms bonded to C atoms have been omitted. Cl atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions ($x, y - 1, z$) and ($x, y + 1, z$), respectively.

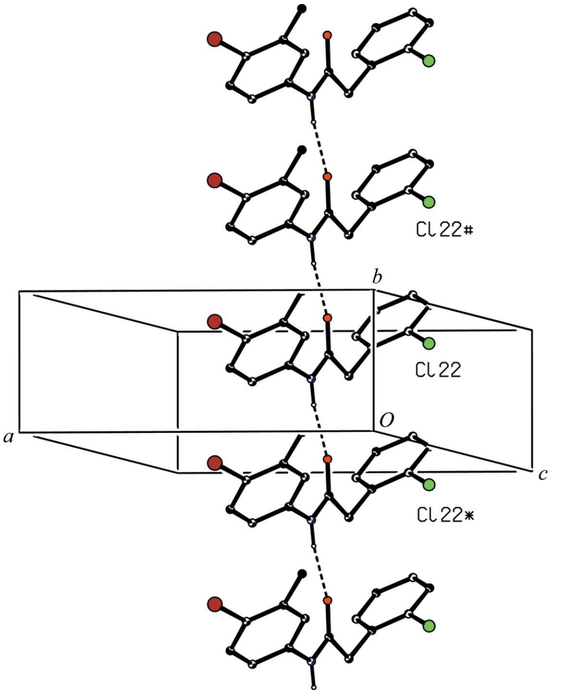


Figure 7
Part of the crystal structure of compound (IV), showing the formation of a $C(4)$ hydrogen-bonded chain parallel to [010]. Hydrogen bonds are shown as dashed lines and, for the sake of clarity, H atoms bonded to C atoms have been omitted. Cl atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions (x, $y - 1$, z) and (x, $y + 1$, z), respectively.

rather than chains of rings; again, there are no direction-specific interactions between adjacent chains.

In the structure of compound (IV), there is a short intermolecular Br$\cdots$Br contact between inversion-related molecules, with Br14$\cdots$Br14$^{\rm i}$ = 3.4303 (8) Å and C14—Br14$\cdots$Br14$^{\rm i}$ = 158.60 (13)° [symmetry code: (i) $-x + 1, -y + 2, -z$]. A database study of the angular distribution of such contacts (Ramasubbu *et al.*, 1986) has shown that the C—$X\cdots X$ angles (where X = Cl, Br or I) are clustered either around 100° or around 165°, and the angle observed in compound (IV) is consistent with this finding. Although the observed Br$\cdots$Br distance in (IV) is shorter that the conventional sum of van der Waals radii (3.70 Å; Rowland & Taylor, 1996), a database study of the nonbonded distances in such contacts (Nyburg & Faerman, 1985) found that atoms such as halogens bonded to C atoms do not behave in this context as though they were spherical, but instead they behave as oblate ellipsoids, with the major axis normal to the direction of the C—X bond and the minor axis parallel to the C—X bond. For Br, these characteristic radii were found to be 2.01 and 1.64 Å, respectively, and, on this basis, the observed Br$\cdots$Br distance in compound (IV) does not seem to be exceptional.

Simple $C(4)$ chains containing molecules related by translation are also found in compounds (V)–(VII). In compound (V) (Fun, Shahani *et al.*, 2012), the chains run parallel to [010] in $P2_1/c$, as in (IV), while in isostructural compounds (VI) and (VII) (Praveen *et al.*, 2013*a*,*b*) the chains run parallel to the [100] direction.

Unlike compounds (I) and (II), compounds (VIII) (Fun, Quah *et al.*, 2012) and (IX) (Fun *et al.*, 2011*a*) (see Scheme 2) are not isostructural, although in each pair the analogues differ only in that compounds (II) and (IX) contain a bromo substituent in place of the chloro substituent in each of compounds (I) and (VIII). Compounds (VIII) and (IX) crystallize in the space groups $P2_1/c$ and $Pbca$, respectively, and, whereas in (VIII) molecules related by translation are linked into simple $C(4)$ chains by N—H$\cdots$O hydrogen bonds, in (IX) molecules related by a b-glide plane are linked by N—H$\cdots$O hydrogen bonds modestly reinforced by C—H$\cdots$O hydrogen bonds to form a $C(4)C(4)[R_2^1(6)]$ chain of rings.

In each of compounds (X) (Praveen *et al.*, 2011) and (XI) (Fun *et al.*, 2011*b*), molecules related by n-glide and c-glide

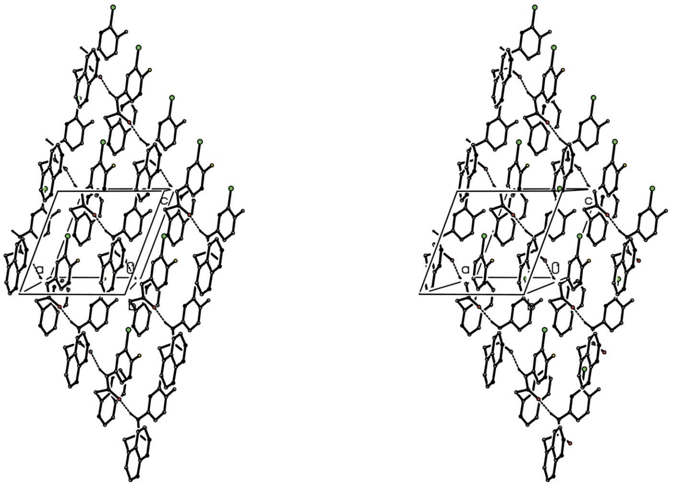


Figure 8
A stereoview of part of the crystal structure of compound (X), showing the formation of a π-stacked sheet of hydrogen-bonded chains parallel to (010). The original atomic coordinates (Praveen *et al.*, 2011) have been used. Hydrogen bonds are shown as dashed lines and, for the sake of clarity, H atoms not involved in the motif shown have been omitted.

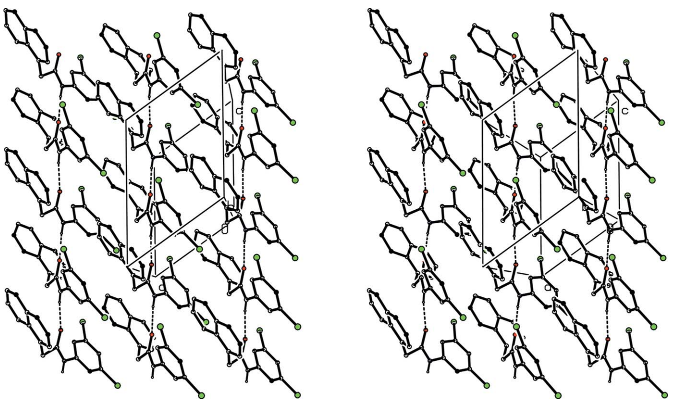


Figure 9
A stereoview of part of the crystal structure of compound (XI), showing the formation of a π-stacked sheet of hydrogen-bonded chains parallel to (010). The original atomic coordinates (Fun *et al.*, 2011*b*) have been used. Hydrogen bonds are shown as dashed lines and, for the sake of clarity, H atoms not involved in the motif shown have been omitted.

planes, respectively, are linked by N—H···O hydrogen bonds to form *C*(4) chains running parallel to [101] and [001] respectively. In addition, there are two aromatic *π*–*π* stacking interactions in each structure, although these were not mentioned in the original structure reports. In each case, one such interaction reinforces the hydrogen-bonded chains and the other links these chains into sheets which lie parallel to (010) in both structures (Figs. 8 and 9).

The *C*(4) motif found in compounds (I)–(XI) appears to be characteristic of amides containing only hydrocarbyl substituents from which other potential hydrogen-bond acceptors are absent (Kashino *et al.*, 1979; Bowes *et al.*, 2003; Glidewell *et al.*, 2003; Kumar *et al.*, 2004; Garden *et al.*, 2005; Cuffini *et al.*, 2006; Wardell *et al.*, 2006). It is noteworthy that in each of compounds (I)–(VII) the repeat vector parallel to the direction of the chain is short, ranging from b = 4.7282 (3) Å in compound (IV) to a = 5.0039 (7) Å in compound (I), and this behaviour is also found in compound (VIII), where b = 5.0458 (11) Å. However, in the other naphthalenyl derivatives, *i.e.* compounds (IX)–(XI), the repeat distance parallel to the chain direction is very much longer (>9 Å in each case) and in each the chain consists of molecules related by glide planes, rather than by pure translation as in compounds (I)–(VIII).

When, however, the *N*-aryl group is replaced by a nitrogen-containing heterocyclic unit (Nayak *et al.*, 2013, 2013*a*,*b*,*c*), N—H···O hydrogen bonds are absent from the structures and the supramolecular assembly is determined by N—H···N hydrogen bonds together with some combination of C—H···N and C—H···O hydrogen bonds and, in some cases, *π*–*π* stacking interactions. An exception is provided by the pyrimidine derivative, *N*-(4,6-dimethoxypyrimidin-2-yl)-2-(3-methylphenyl)acetamide (Praveen *et al.*, 2012); this is an example of a *cis*-amide (although, unfortunately, the schematic diagram in the original structure report depicts this as a *trans*-amide) and inversion-related pairs of N—H···O hydrogen bonds link pairs of molecules into centrosymmetric $R_2^2(8)$ dimers.

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References

Agilent (2012). *CrysAlis PRO* and *CrysAlis RED*. Agilent Technologies Ltd, Yarnton, Oxfordshire, England.

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Bowes, K. F., Glidewell, C., Low, J. N., Skakle, J. M. S. & Wardell, J. L. (2003). *Acta Cryst.* C**59**, o1–o3.

Csöregh, I. & Palm, T.-B. (1977). *Acta Cryst.* B**33**, 2169–2175.

Cuffini, S., Glidewell, C., Low, J. N., de Oliveira, A. G., de Souza, M. V. N., Vasconcelos, T. R. A., Wardell, S. M. S. V. & Wardell, J. L. (2006). *Acta Cryst.* B**62**, 651–665.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Fun, H.-K., Quah, C. K., Narayana, B., Nayak, P. S. & Sarojini, B. K. (2011*a*). *Acta Cryst.* E**67**, o2926–o2927.

Fun, H.-K., Quah, C. K., Narayana, B., Nayak, P. S. & Sarojini, B. K. (2011*b*). *Acta Cryst.* E**67**, o2941–o2942.

Fun, H.-K., Quah, C. K., Nayak, P. S., Narayana, B. & Sarojini, B. K. (2012). *Acta Cryst.* E**68**, o2463.

Fun, H.-K., Shahani, T., Nayak, P. S., Narayana, B. & Sarojini, B. K. (2012). *Acta Cryst.* E**68**, o519.

Garden, S. J., Glidewell, C., Low, J. N., Skakle, J. M. S. & Wardell, J. L. (2005). *Acta Cryst.* C**61**, o450–o451.

Glidewell, C., Low, J. N., Skakle, J. M. S. & Wardell, J. L. (2003). *Acta Cryst.* C**59**, o636–o637.

Kashino, S., Ito, K. & Haisa, M. (1979). *Bull. Chem. Soc. Jpn*, **52**, 365–369.

Kojić-Prodić, B. & Ružoć-Toroš, Ž. (1978). *Acta Cryst.* B**34**, 1271–1275.

Kumar, D. K., Jose, D. A., Dastidar, P. & Das, A. (2004). *Langmuir*, **20**, 10413–10418.

Mijin, D. & Marinkovic, A. (2006). *Synth. Commun.* **36**, 193–198.

Mijin, D. Z., Prascevic, M. & Petrovic, S. D. (2008). *J. Serb. Chem. Soc.* **73**, 945–950.

Nayak, P. S., Narayana, B., Jasinski, J. P., Yathirajan, H. S. & Sarojini, B. K. (2013). *Acta Cryst.* E**69**, o891.

Nayak, P. S., Narayana, B., Yathirajan, H. S., Jasinski, J. P. & Butcher, R. J. (2013*a*). *Acta Cryst.* E**69**, o523.

Nayak, P. S., Narayana, B., Yathirajan, H. S., Jasinski, J. P. & Butcher, R. J. (2013*b*). *Acta Cryst.* E**69**, o645–o646.

Nayak, P. S., Narayana, B., Yathirajan, H. S., Jasinski, J. P. & Butcher, R. J. (2013*c*). *Acta Cryst.* E**69**, o656–o657.

Nyburg, S. C. & Faerman, C. H. (1985). *Acta Cryst.* B**41**, 274–279.

Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.

Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.

Pitt, G. J. (1952). *Acta Cryst.* **5**, 770–775.

Praveen, A. S., Jasinski, J. P., Golen, J. A., Narayana, B. & Yathirajan, H. S. (2011). *Acta Cryst.* E**67**, o1826.

Praveen, A. S., Jasinski, J. P., Golen, J. A., Yathirajan, H. S. & Narayana, B. (2012). *Acta Cryst.* E**68**, o226–o227.

Praveen, A. S., Yathirajan, H. S., Jasinski, J. P., Keeley, A. C., Narayana, B. & Sarojini, B. K. (2013*a*). *Acta Cryst.* E**69**, o900–o901.

Praveen, A. S., Yathirajan, H. S., Jasinski, J. P., Keeley, A. C., Narayana, B. & Sarojini, B. K. (2013*b*). *Acta Cryst.* E**69**, o996–o997.

Ramasubbu, N., Parthasarathy, R. & Murray-Rust, P. (1986). *J. Am. Chem. Soc.* **108**, 4308–4314.

Rowland, R. S. & Taylor, R. (1996). *J. Phys. Chem.* **100**, 7384–7391.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2014). *SHELXL2014*. University of Göttingen, Germany.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Wardell, J. L., Low, J. N., Skakle, J. M. S. & Glidewell, C. (2006). *Acta Cryst.* B**62**, 931–943.

supporting information

Acta Cryst. (2014). C**70**, 889-894   [doi:10.1107/S2053229614018713]

Halogenated *C*,*N*-diarylacetamides: molecular conformations and supramolecular assembly

Prakash S. Nayak, Jerry P. Jasinski, James A. Golen, Badiadka Narayana, Manpreet Kaur, Hemmige S. Yathirajan and Christopher Glidewell

Computing details

For all compounds, data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: SUPERFLIP (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2014); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2014) and *PLATON* (Spek, 2009).

(I) *N*-(4-Chloro-3-methylphenyl)-2-phenylacetamide

Crystal data

$C_{15}H_{14}ClNO$
$M_r = 259.72$
Triclinic, $P\overline{1}$
$a = 5.0039$ (7) Å
$b = 10.7525$ (12) Å
$c = 12.6177$ (12) Å
$\alpha = 108.615$ (10)°
$\beta = 91.771$ (11)°
$\gamma = 90.167$ (11)°
$V = 643.01$ (14) Å^3

$Z = 2$
$F(000) = 272$
$D_x = 1.342$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2447 reflections
$\theta = 3.7$–$72.4°$
$\mu = 2.51$ mm^{-1}
$T = 173$ K
Block, colourless
0.28 × 0.16 × 0.08 mm

Data collection

Agilent Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{\min} = 0.413$, $T_{\max} = 0.818$
3772 measured reflections

2447 independent reflections
1865 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.032$
$\theta_{\max} = 72.4°$, $\theta_{\min} = 3.7°$
$h = -6 \rightarrow 5$
$k = -13 \rightarrow 12$
$l = -11 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.187$
$S = 1.09$
2447 reflections
164 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-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.093P)^2 + 0.0997P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2965 (6)	0.7657 (3)	0.5498 (3)	0.0381 (7)
O1	0.0598 (4)	0.7371 (2)	0.5294 (2)	0.0474 (6)
N1	0.4929 (5)	0.7032 (2)	0.4826 (2)	0.0382 (6)
H1	0.6572	0.7331	0.5018	0.046*
C2	0.3951 (6)	0.8735 (3)	0.6541 (3)	0.0476 (8)
H2A	0.4673	0.8326	0.7089	0.057*
H2B	0.5436	0.9219	0.6341	0.057*
C11	0.4580 (6)	0.5937 (3)	0.3837 (2)	0.0352 (6)
C12	0.6223 (6)	0.5854 (3)	0.2949 (3)	0.0412 (7)
H12	0.7489	0.6539	0.3022	0.049*
C13	0.6082 (6)	0.4808 (3)	0.1961 (3)	0.0406 (7)
C14	0.4197 (6)	0.3831 (3)	0.1900 (3)	0.0410 (7)
Cl14	0.38569 (19)	0.24733 (8)	0.06853 (7)	0.0578 (3)
C15	0.2555 (7)	0.3892 (3)	0.2774 (3)	0.0440 (7)
H15	0.1298	0.3205	0.2705	0.053*
C16	0.2731 (6)	0.4949 (3)	0.3751 (3)	0.0395 (7)
H16	0.1599	0.4995	0.4353	0.047*
C17	0.7884 (7)	0.4765 (4)	0.1016 (3)	0.0578 (9)
H17A	0.6812	0.4862	0.0385	0.087*
H17B	0.8806	0.3923	0.0780	0.087*
H17C	0.9205	0.5483	0.1269	0.087*
C21	0.1835 (6)	0.9697 (3)	0.7089 (3)	0.0398 (7)
C22	0.0824 (7)	0.9718 (3)	0.8102 (3)	0.0450 (7)
H22	0.1475	0.9119	0.8459	0.054*
C23	−0.1131 (7)	1.0605 (3)	0.8601 (3)	0.0523 (9)
H23	−0.1815	1.0603	0.9294	0.063*
C24	−0.2089 (7)	1.1487 (3)	0.8104 (3)	0.0498 (8)
H24	−0.3424	1.2095	0.8450	0.060*
C25	−0.1088 (7)	1.1479 (3)	0.7095 (3)	0.0493 (8)
H25	−0.1742	1.2082	0.6742	0.059*
C26	0.0868 (7)	1.0597 (3)	0.6596 (3)	0.0459 (8)
H26	0.1558	1.0607	0.5906	0.055*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0324 (16)	0.0370 (14)	0.0442 (17)	0.0064 (12)	0.0039 (12)	0.0117 (13)
O1	0.0277 (11)	0.0470 (12)	0.0580 (14)	0.0048 (9)	0.0050 (9)	0.0031 (10)
N1	0.0247 (12)	0.0414 (13)	0.0483 (15)	0.0039 (10)	0.0039 (10)	0.0140 (11)
C2	0.0345 (17)	0.0472 (17)	0.054 (2)	0.0058 (13)	−0.0031 (14)	0.0061 (15)
C11	0.0292 (14)	0.0379 (14)	0.0407 (15)	0.0127 (11)	0.0041 (11)	0.0152 (12)
C12	0.0323 (16)	0.0466 (17)	0.0504 (18)	0.0067 (12)	0.0068 (13)	0.0230 (15)
C13	0.0347 (16)	0.0516 (17)	0.0406 (16)	0.0156 (13)	0.0072 (12)	0.0211 (14)
C14	0.0427 (17)	0.0415 (16)	0.0389 (16)	0.0155 (13)	0.0063 (13)	0.0125 (13)
Cl14	0.0660 (6)	0.0503 (5)	0.0489 (5)	0.0115 (4)	0.0099 (4)	0.0033 (4)
C15	0.0432 (18)	0.0374 (15)	0.0531 (19)	0.0048 (13)	0.0083 (14)	0.0160 (14)
C16	0.0359 (16)	0.0404 (15)	0.0458 (17)	0.0091 (12)	0.0103 (13)	0.0181 (14)
C17	0.050 (2)	0.075 (2)	0.053 (2)	0.0121 (18)	0.0143 (16)	0.0248 (19)
C21	0.0340 (16)	0.0347 (14)	0.0456 (17)	0.0002 (12)	−0.0002 (13)	0.0059 (13)
C22	0.0482 (19)	0.0437 (17)	0.0441 (18)	0.0057 (14)	−0.0015 (14)	0.0159 (14)
C23	0.056 (2)	0.055 (2)	0.0402 (18)	0.0023 (16)	0.0084 (15)	0.0066 (15)
C24	0.0439 (19)	0.0393 (16)	0.056 (2)	0.0086 (14)	0.0053 (15)	−0.0002 (15)
C25	0.0466 (19)	0.0383 (16)	0.064 (2)	0.0072 (14)	−0.0011 (16)	0.0180 (15)
C26	0.0455 (18)	0.0460 (17)	0.0480 (18)	0.0017 (14)	0.0054 (14)	0.0174 (15)

Geometric parameters (Å, º)

C1—O1	1.221 (4)	C15—H15	0.9500
C1—N1	1.352 (4)	C16—H16	0.9500
C1—C2	1.517 (4)	C17—H17A	0.9800
N1—C11	1.422 (4)	C17—H17B	0.9800
N1—H1	0.8800	C17—H17C	0.9800
C2—C21	1.505 (4)	C21—C22	1.383 (5)
C2—H2A	0.9900	C21—C26	1.387 (5)
C2—H2B	0.9900	C22—C23	1.387 (4)
C11—C16	1.382 (4)	C22—H22	0.9500
C11—C12	1.391 (4)	C23—C24	1.373 (5)
C12—C13	1.386 (4)	C23—H23	0.9500
C12—H12	0.9500	C24—C25	1.379 (5)
C13—C14	1.392 (5)	C24—H24	0.9500
C13—C17	1.506 (4)	C25—C26	1.385 (5)
C14—C15	1.381 (4)	C25—H25	0.9500
C14—Cl14	1.750 (3)	C26—H26	0.9500
C15—C16	1.385 (4)		
O1—C1—N1	123.1 (3)	C11—C16—C15	119.0 (3)
O1—C1—C2	122.6 (3)	C11—C16—H16	120.5
N1—C1—C2	114.3 (3)	C15—C16—H16	120.5
C1—N1—C11	125.9 (2)	C13—C17—H17A	109.5
C1—N1—H1	117.0	C13—C17—H17B	109.5
C11—N1—H1	117.0	H17A—C17—H17B	109.5

C21—C2—C1	114.1 (3)	C13—C17—H17C	109.5
C21—C2—H2A	108.7	H17A—C17—H17C	109.5
C1—C2—H2A	108.7	H17B—C17—H17C	109.5
C21—C2—H2B	108.7	C22—C21—C26	118.2 (3)
C1—C2—H2B	108.7	C22—C21—C2	120.9 (3)
H2A—C2—H2B	107.6	C26—C21—C2	120.8 (3)
C16—C11—C12	119.8 (3)	C21—C22—C23	120.6 (3)
C16—C11—N1	122.1 (3)	C21—C22—H22	119.7
C12—C11—N1	118.1 (3)	C23—C22—H22	119.7
C13—C12—C11	122.4 (3)	C24—C23—C22	120.7 (3)
C13—C12—H12	118.8	C24—C23—H23	119.6
C11—C12—H12	118.8	C22—C23—H23	119.6
C12—C13—C14	116.4 (3)	C23—C24—C25	119.2 (3)
C12—C13—C17	120.6 (3)	C23—C24—H24	120.4
C14—C13—C17	123.0 (3)	C25—C24—H24	120.4
C15—C14—C13	122.1 (3)	C24—C25—C26	120.3 (3)
C15—C14—Cl14	118.0 (3)	C24—C25—H25	119.9
C13—C14—Cl14	119.9 (2)	C26—C25—H25	119.9
C14—C15—C16	120.4 (3)	C25—C26—C21	121.0 (3)
C14—C15—H15	119.8	C25—C26—H26	119.5
C16—C15—H15	119.8	C21—C26—H26	119.5

O1—C1—N1—C11	−3.2 (5)	Cl14—C14—C15—C16	−179.6 (2)
C2—C1—N1—C11	175.8 (3)	C12—C11—C16—C15	−0.1 (4)
O1—C1—C2—C21	−19.4 (5)	N1—C11—C16—C15	−178.1 (3)
N1—C1—C2—C21	161.5 (3)	C14—C15—C16—C11	−0.3 (5)
C1—N1—C11—C16	−37.5 (4)	C1—C2—C21—C22	109.2 (4)
C1—N1—C11—C12	144.4 (3)	C1—C2—C21—C26	−71.5 (4)
C16—C11—C12—C13	0.2 (4)	C26—C21—C22—C23	0.9 (5)
N1—C11—C12—C13	178.4 (3)	C2—C21—C22—C23	−179.8 (3)
C11—C12—C13—C14	−0.1 (4)	C21—C22—C23—C24	−0.5 (5)
C11—C12—C13—C17	179.4 (3)	C22—C23—C24—C25	0.2 (5)
C12—C13—C14—C15	−0.2 (4)	C23—C24—C25—C26	−0.3 (5)
C17—C13—C14—C15	−179.7 (3)	C24—C25—C26—C21	0.7 (5)
C12—C13—C14—Cl14	179.8 (2)	C22—C21—C26—C25	−1.0 (5)
C17—C13—C14—Cl14	0.3 (4)	C2—C21—C26—C25	179.7 (3)
C13—C14—C15—C16	0.4 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	2.03	2.878 (3)	161
C2—H2*B*···*Cg*1^{i}	0.99	2.81	3.546 (4)	132

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

(II) *N*-(4-Bromo-3-methylphenyl)-2-phenylacetamide

Crystal data

$C_{15}H_{14}BrNO$
M_r = 304.18
Triclinic, $P\overline{1}$
a = 4.9995 (3) Å
b = 10.8392 (4) Å
c = 12.7301 (7) Å
α = 108.149 (4)°
β = 91.968 (5)°
γ = 90.310 (4)°
V = 655.05 (6) Å^3
Z = 2
F(000) = 308
D_x = 1.542 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 2515 reflections
θ = 4.3–72.4°
μ = 4.16 mm^{-1}
T = 173 K
Plate, colourless
0.32 × 0.18 × 0.08 mm

Data collection

Agilent Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.286, T_{max} = 0.818
3876 measured reflections
2515 independent reflections
2276 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 72.4°, θ_{min} = 4.3°
$h = -6 \rightarrow 6$
$k = -13 \rightarrow 8$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.110
S = 1.07
2515 reflections
164 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 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.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.2977 (5)	0.7638 (2)	0.5510 (2)	0.0290 (5)
O1	0.0594 (4)	0.7346 (2)	0.53092 (18)	0.0398 (5)
N1	0.4932 (4)	0.7035 (2)	0.48448 (19)	0.0302 (5)
H1	0.6577	0.7332	0.5037	0.036*
C2	0.3984 (5)	0.8692 (3)	0.6554 (2)	0.0369 (6)
H2A	0.4635	0.8277	0.7104	0.044*
H2B	0.5519	0.9158	0.6370	0.044*
C11	0.4584 (5)	0.5970 (2)	0.3866 (2)	0.0273 (5)
C12	0.6214 (5)	0.5910 (3)	0.2990 (2)	0.0318 (5)
H12	0.7472	0.6595	0.3066	0.038*

C13	0.6073 (5)	0.4886 (3)	0.2008 (2)	0.0334 (5)
C14	0.4191 (5)	0.3906 (3)	0.1937 (2)	0.0315 (5)
Br14	0.37906 (7)	0.24603 (3)	0.06240 (2)	0.04614 (15)
C15	0.2543 (6)	0.3946 (3)	0.2798 (2)	0.0341 (6)
H15	0.1284	0.3261	0.2723	0.041*
C16	0.2720 (5)	0.4974 (3)	0.3765 (2)	0.0319 (5)
H16	0.1586	0.5003	0.4356	0.038*
C17	0.7862 (7)	0.4883 (4)	0.1079 (3)	0.0470 (7)
H17A	0.8685	0.4031	0.0793	0.071*
H17B	0.9266	0.5552	0.1356	0.071*
H17C	0.6801	0.5066	0.0485	0.071*
C21	0.1876 (5)	0.9661 (3)	0.7065 (2)	0.0307 (5)
C22	0.0826 (6)	0.9695 (3)	0.8069 (2)	0.0371 (6)
H22	0.1438	0.9100	0.8432	0.045*
C23	−0.1117 (6)	1.0592 (3)	0.8550 (2)	0.0422 (7)
H23	−0.1816	1.0606	0.9238	0.051*
C24	−0.2022 (6)	1.1455 (3)	0.8029 (3)	0.0423 (7)
H24	−0.3340	1.2069	0.8357	0.051*
C25	−0.1001 (6)	1.1423 (3)	0.7023 (3)	0.0405 (6)
H25	−0.1631	1.2013	0.6658	0.049*
C26	0.0933 (6)	1.0535 (3)	0.6548 (2)	0.0365 (6)
H26	0.1624	1.0524	0.5860	0.044*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0263 (12)	0.0263 (12)	0.0337 (13)	0.0012 (9)	0.0029 (9)	0.0081 (10)
O1	0.0231 (9)	0.0364 (11)	0.0489 (11)	0.0001 (7)	0.0038 (8)	−0.0030 (9)
N1	0.0219 (9)	0.0298 (11)	0.0374 (11)	−0.0007 (8)	0.0013 (8)	0.0083 (9)
C2	0.0277 (12)	0.0361 (14)	0.0400 (14)	0.0011 (11)	−0.0006 (11)	0.0018 (12)
C11	0.0239 (11)	0.0267 (12)	0.0321 (12)	0.0041 (9)	0.0025 (9)	0.0101 (10)
C12	0.0253 (12)	0.0339 (14)	0.0392 (14)	−0.0009 (10)	0.0041 (10)	0.0154 (11)
C13	0.0306 (12)	0.0370 (14)	0.0360 (13)	0.0078 (10)	0.0059 (10)	0.0154 (11)
C14	0.0389 (14)	0.0253 (12)	0.0285 (12)	0.0072 (10)	0.0040 (10)	0.0054 (10)
Br14	0.0619 (3)	0.0346 (2)	0.0363 (2)	0.00613 (14)	0.00912 (14)	0.00200 (13)
C15	0.0375 (14)	0.0265 (13)	0.0382 (14)	−0.0001 (10)	0.0059 (11)	0.0093 (11)
C16	0.0337 (13)	0.0294 (13)	0.0349 (13)	0.0026 (10)	0.0106 (10)	0.0123 (11)
C17	0.0439 (16)	0.060 (2)	0.0400 (16)	0.0038 (14)	0.0135 (13)	0.0182 (14)
C21	0.0284 (12)	0.0254 (12)	0.0342 (13)	−0.0027 (10)	−0.0001 (10)	0.0035 (10)
C22	0.0436 (15)	0.0334 (14)	0.0337 (14)	−0.0008 (11)	−0.0008 (11)	0.0097 (11)
C23	0.0469 (17)	0.0439 (17)	0.0299 (13)	0.0004 (13)	0.0076 (12)	0.0020 (12)
C24	0.0405 (15)	0.0307 (14)	0.0472 (16)	0.0035 (11)	0.0048 (12)	−0.0008 (12)
C25	0.0445 (15)	0.0270 (14)	0.0509 (17)	0.0006 (11)	−0.0022 (13)	0.0137 (12)
C26	0.0389 (14)	0.0356 (14)	0.0364 (14)	−0.0040 (11)	0.0058 (11)	0.0127 (11)

Geometric parameters (Å, º)

C1—O1	1.228 (3)	C15—H15	0.9500
C1—N1	1.348 (3)	C16—H16	0.9500
C1—C2	1.526 (4)	C17—H17A	0.9800
N1—C11	1.415 (3)	C17—H17B	0.9800
N1—H1	0.8800	C17—H17C	0.9800
C2—C21	1.507 (4)	C21—C26	1.387 (4)
C2—H2A	0.9900	C21—C22	1.388 (4)
C2—H2B	0.9900	C22—C23	1.394 (4)
C11—C12	1.389 (4)	C22—H22	0.9500
C11—C16	1.395 (4)	C23—C24	1.375 (5)
C12—C13	1.389 (4)	C23—H23	0.9500
C12—H12	0.9500	C24—C25	1.385 (5)
C13—C14	1.394 (4)	C24—H24	0.9500
C13—C17	1.506 (4)	C25—C26	1.383 (4)
C14—C15	1.384 (4)	C25—H25	0.9500
C14—Br14	1.905 (3)	C26—H26	0.9500
C15—C16	1.379 (4)		
O1—C1—N1	123.2 (2)	C15—C16—C11	119.2 (2)
O1—C1—C2	122.6 (2)	C15—C16—H16	120.4
N1—C1—C2	114.2 (2)	C11—C16—H16	120.4
C1—N1—C11	126.1 (2)	C13—C17—H17A	109.5
C1—N1—H1	117.0	C13—C17—H17B	109.5
C11—N1—H1	117.0	H17A—C17—H17B	109.5
C21—C2—C1	113.3 (2)	C13—C17—H17C	109.5
C21—C2—H2A	108.9	H17A—C17—H17C	109.5
C1—C2—H2A	108.9	H17B—C17—H17C	109.5
C21—C2—H2B	108.9	C26—C21—C22	118.4 (3)
C1—C2—H2B	108.9	C26—C21—C2	121.2 (3)
H2A—C2—H2B	107.7	C22—C21—C2	120.4 (3)
C12—C11—C16	119.4 (2)	C21—C22—C23	120.8 (3)
C12—C11—N1	118.2 (2)	C21—C22—H22	119.6
C16—C11—N1	122.3 (2)	C23—C22—H22	119.6
C11—C12—C13	122.4 (2)	C24—C23—C22	120.0 (3)
C11—C12—H12	118.8	C24—C23—H23	120.0
C13—C12—H12	118.8	C22—C23—H23	120.0
C12—C13—C14	116.6 (2)	C23—C24—C25	119.6 (3)
C12—C13—C17	120.1 (3)	C23—C24—H24	120.2
C14—C13—C17	123.3 (3)	C25—C24—H24	120.2
C15—C14—C13	122.0 (3)	C26—C25—C24	120.3 (3)
C15—C14—Br14	117.6 (2)	C26—C25—H25	119.9
C13—C14—Br14	120.4 (2)	C24—C25—H25	119.9
C16—C15—C14	120.4 (2)	C25—C26—C21	120.8 (3)
C16—C15—H15	119.8	C25—C26—H26	119.6
C14—C15—H15	119.8	C21—C26—H26	119.6

O1—C1—N1—C11	−2.7 (4)	Br14—C14—C15—C16	−179.4 (2)
C2—C1—N1—C11	175.6 (2)	C14—C15—C16—C11	−0.2 (4)
O1—C1—C2—C21	−22.5 (4)	C12—C11—C16—C15	0.3 (4)
N1—C1—C2—C21	159.1 (2)	N1—C11—C16—C15	−178.1 (2)
C1—N1—C11—C12	144.2 (3)	C1—C2—C21—C26	−69.4 (3)
C1—N1—C11—C16	−37.4 (4)	C1—C2—C21—C22	110.5 (3)
C16—C11—C12—C13	−0.3 (4)	C26—C21—C22—C23	−0.4 (4)
N1—C11—C12—C13	178.2 (2)	C2—C21—C22—C23	179.7 (3)
C11—C12—C13—C14	0.1 (4)	C21—C22—C23—C24	0.2 (4)
C11—C12—C13—C17	179.1 (3)	C22—C23—C24—C25	0.3 (5)
C12—C13—C14—C15	−0.1 (4)	C23—C24—C25—C26	−0.5 (5)
C17—C13—C14—C15	−178.9 (3)	C24—C25—C26—C21	0.2 (4)
C12—C13—C14—Br14	179.40 (18)	C22—C21—C26—C25	0.2 (4)
C17—C13—C14—Br14	0.5 (4)	C2—C21—C26—C25	−179.9 (3)
C13—C14—C15—C16	0.1 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	2.03	2.868 (3)	160
C2—H2*B*···*Cg*1^{i}	0.99	2.78	3.546 (3)	135

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

(III) *N*-(4-Chloro-3-methylphenyl)-2-(2,4-dichlorophenyl)acetamide

Crystal data

$C_{15}H_{12}Cl_3NO$
$M_r = 328.61$
Monoclinic, $P2_1$
$a = 11.8441 (7)$ Å
$b = 4.7288 (3)$ Å
$c = 13.0981 (7)$ Å
$\beta = 101.310 (6)$°
$V = 719.36 (7)$ Å^3
$Z = 2$

$F(000) = 336$
$D_x = 1.517$ Mg m^{-3}
Cu *Kα* radiation, $\lambda = 1.54184$ Å
Cell parameters from 2566 reflections
$\theta = 3.4$–72.2°
$\mu = 5.71$ mm^{-1}
$T = 173$ K
Block, colourless
0.16 × 0.08 × 0.06 mm

Data collection

Agilent Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min} = 0.256$, $T_{max} = 0.710$
4196 measured reflections

2566 independent reflections
2214 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 72.2°$, $\theta_{min} = 3.4°$
$h = -7 \rightarrow 14$
$k = -5 \rightarrow 5$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.155$
$S = 1.07$

2566 reflections
182 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.074P)^2 + 0.1558P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Absolute structure: Flack *x* determined using 697 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.02 (4)

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_{iso}*/U_{eq}
C1	0.2642 (5)	0.4768 (13)	0.5713 (5)	0.0269 (12)
O1	0.2599 (4)	0.7328 (11)	0.5588 (4)	0.0396 (11)
N1	0.2985 (4)	0.2962 (11)	0.5045 (4)	0.0279 (11)
H1	0.2980	0.1145	0.5189	0.034*
C2	0.2333 (7)	0.3377 (15)	0.6672 (5)	0.0374 (15)
H2A	0.1727	0.1939	0.6448	0.045*
H2B	0.3020	0.2398	0.7069	0.045*
C11	0.3360 (5)	0.3802 (13)	0.4110 (5)	0.0260 (12)
C12	0.2736 (5)	0.5755 (14)	0.3438 (5)	0.0288 (12)
H12	0.2065	0.6576	0.3608	0.035*
C13	0.3077 (5)	0.6540 (14)	0.2516 (5)	0.0317 (14)
C14	0.4081 (5)	0.5313 (18)	0.2321 (5)	0.0383 (16)
Cl14	0.45559 (16)	0.6230 (6)	0.11761 (14)	0.0585 (7)
C15	0.4702 (6)	0.3367 (18)	0.2978 (5)	0.0409 (16)
H15	0.5377	0.2550	0.2814	0.049*
C16	0.4341 (6)	0.2593 (16)	0.3887 (5)	0.0367 (15)
H16	0.4766	0.1248	0.4348	0.044*
C17	0.2369 (7)	0.8607 (18)	0.1784 (6)	0.0434 (17)
H17A	0.2041	0.7649	0.1130	0.065*
H17B	0.2860	1.0171	0.1644	0.065*
H17C	0.1746	0.9347	0.2102	0.065*
C21	0.1914 (5)	0.5477 (14)	0.7367 (5)	0.0311 (13)
C22	0.0803 (6)	0.6557 (13)	0.7175 (5)	0.0323 (14)
Cl22	−0.01755 (16)	0.5362 (5)	0.60924 (14)	0.0496 (5)
C23	0.0429 (6)	0.8549 (15)	0.7797 (5)	0.0327 (13)
H23	−0.0341	0.9223	0.7644	0.039*
C24	0.1211 (6)	0.9555 (13)	0.8660 (5)	0.0310 (14)
Cl24	0.07578 (15)	1.2083 (4)	0.94506 (12)	0.0401 (4)
C25	0.2322 (6)	0.8551 (16)	0.8878 (5)	0.0336 (14)
H25	0.2854	0.9257	0.9461	0.040*
C26	0.2663 (5)	0.6515 (14)	0.8247 (5)	0.0333 (15)
H26	0.3426	0.5798	0.8416	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.031 (3)	0.022 (3)	0.028 (3)	−0.003 (2)	0.009 (2)	0.002 (2)
O1	0.062 (3)	0.024 (2)	0.038 (2)	−0.001 (2)	0.022 (2)	0.002 (2)
N1	0.035 (3)	0.019 (2)	0.030 (3)	−0.001 (2)	0.010 (2)	0.001 (2)
C2	0.052 (4)	0.029 (3)	0.035 (3)	0.001 (3)	0.020 (3)	0.006 (3)
C11	0.027 (3)	0.023 (3)	0.027 (3)	0.000 (2)	0.004 (2)	−0.003 (2)
C12	0.028 (3)	0.029 (3)	0.030 (3)	0.001 (3)	0.007 (2)	−0.003 (3)
C13	0.029 (3)	0.036 (4)	0.029 (3)	−0.001 (2)	0.004 (2)	0.003 (3)
C14	0.035 (3)	0.056 (5)	0.026 (3)	−0.004 (3)	0.011 (2)	0.003 (3)
Cl14	0.0456 (9)	0.0954 (18)	0.0388 (8)	0.0073 (10)	0.0183 (7)	0.0197 (10)
C15	0.032 (3)	0.055 (4)	0.038 (3)	0.010 (3)	0.014 (3)	0.000 (3)
C16	0.037 (3)	0.039 (4)	0.033 (3)	0.004 (3)	0.006 (3)	0.008 (3)
C17	0.046 (4)	0.049 (4)	0.036 (3)	0.007 (3)	0.007 (3)	0.012 (3)
C21	0.041 (3)	0.024 (3)	0.032 (3)	−0.004 (3)	0.017 (2)	0.007 (3)
C22	0.040 (3)	0.029 (4)	0.028 (3)	−0.010 (3)	0.006 (2)	0.008 (3)
Cl22	0.0483 (10)	0.0577 (12)	0.0400 (9)	−0.0107 (9)	0.0018 (7)	−0.0027 (9)
C23	0.036 (3)	0.029 (3)	0.036 (3)	0.002 (3)	0.013 (3)	0.005 (3)
C24	0.042 (3)	0.023 (3)	0.033 (3)	0.002 (3)	0.021 (3)	0.004 (2)
Cl24	0.0554 (10)	0.0309 (8)	0.0406 (8)	0.0052 (7)	0.0257 (7)	0.0016 (7)
C25	0.038 (3)	0.037 (4)	0.028 (3)	−0.005 (3)	0.011 (3)	0.003 (3)
C26	0.032 (3)	0.037 (4)	0.033 (3)	0.002 (3)	0.010 (2)	0.011 (3)

Geometric parameters (Å, º)

C1—O1	1.221 (8)	C15—H15	0.9500
C1—N1	1.341 (8)	C16—H16	0.9500
C1—C2	1.526 (8)	C17—H17A	0.9800
N1—C11	1.439 (7)	C17—H17B	0.9800
N1—H1	0.8800	C17—H17C	0.9800
C2—C21	1.495 (9)	C21—C22	1.387 (9)
C2—H2A	0.9900	C21—C26	1.399 (9)
C2—H2B	0.9900	C22—C23	1.375 (9)
C11—C16	1.377 (9)	C22—Cl22	1.740 (6)
C11—C12	1.385 (9)	C23—C24	1.397 (10)
C12—C13	1.397 (8)	C23—H23	0.9500
C12—H12	0.9500	C24—C25	1.376 (9)
C13—C14	1.391 (9)	C24—Cl24	1.734 (6)
C13—C17	1.504 (9)	C25—C26	1.379 (9)
C14—C15	1.372 (11)	C25—H25	0.9500
C14—Cl14	1.756 (6)	C26—H26	0.9500
C15—C16	1.390 (9)		
O1—C1—N1	123.6 (6)	C11—C16—C15	119.1 (6)
O1—C1—C2	121.8 (6)	C11—C16—H16	120.4
N1—C1—C2	114.5 (5)	C15—C16—H16	120.4
C1—N1—C11	124.3 (5)	C13—C17—H17A	109.5

C1—N1—H1	117.9	C13—C17—H17B	109.5
C11—N1—H1	117.9	H17A—C17—H17B	109.5
C21—C2—C1	112.1 (6)	C13—C17—H17C	109.5
C21—C2—H2A	109.2	H17A—C17—H17C	109.5
C1—C2—H2A	109.2	H17B—C17—H17C	109.5
C21—C2—H2B	109.2	C22—C21—C26	116.4 (6)
C1—C2—H2B	109.2	C22—C21—C2	123.4 (6)
H2A—C2—H2B	107.9	C26—C21—C2	120.1 (6)
C16—C11—C12	120.6 (6)	C23—C22—C21	123.3 (6)
C16—C11—N1	118.7 (5)	C23—C22—Cl22	117.7 (5)
C12—C11—N1	120.6 (5)	C21—C22—Cl22	119.0 (5)
C11—C12—C13	121.2 (5)	C22—C23—C24	118.3 (6)
C11—C12—H12	119.4	C22—C23—H23	120.9
C13—C12—H12	119.4	C24—C23—H23	120.9
C14—C13—C12	116.8 (6)	C25—C24—C23	120.4 (6)
C14—C13—C17	122.9 (6)	C25—C24—Cl24	120.6 (6)
C12—C13—C17	120.3 (6)	C23—C24—Cl24	119.0 (5)
C15—C14—C13	122.5 (6)	C24—C25—C26	119.8 (6)
C15—C14—Cl14	118.7 (5)	C24—C25—H25	120.1
C13—C14—Cl14	118.9 (5)	C26—C25—H25	120.1
C14—C15—C16	119.8 (6)	C25—C26—C21	121.8 (6)
C14—C15—H15	120.1	C25—C26—H26	119.1
C16—C15—H15	120.1	C21—C26—H26	119.1

O1—C1—N1—C11	0.9 (10)	N1—C11—C16—C15	179.2 (6)
C2—C1—N1—C11	−177.5 (5)	C14—C15—C16—C11	0.0 (12)
O1—C1—C2—C21	3.8 (10)	C1—C2—C21—C22	79.3 (8)
N1—C1—C2—C21	−177.8 (6)	C1—C2—C21—C26	−98.9 (7)
C1—N1—C11—C16	134.5 (7)	C26—C21—C22—C23	0.2 (9)
C1—N1—C11—C12	−46.5 (9)	C2—C21—C22—C23	−178.0 (6)
C16—C11—C12—C13	0.4 (10)	C26—C21—C22—Cl22	−180.0 (4)
N1—C11—C12—C13	−178.5 (6)	C2—C21—C22—Cl22	1.8 (8)
C11—C12—C13—C14	−1.3 (10)	C21—C22—C23—C24	0.7 (10)
C11—C12—C13—C17	178.3 (6)	Cl22—C22—C23—C24	−179.1 (5)
C12—C13—C14—C15	1.6 (11)	C22—C23—C24—C25	−0.4 (9)
C17—C13—C14—C15	−178.0 (7)	C22—C23—C24—Cl24	179.6 (5)
C12—C13—C14—Cl14	−179.7 (5)	C23—C24—C25—C26	−0.7 (9)
C17—C13—C14—Cl14	0.6 (10)	Cl24—C24—C25—C26	179.2 (5)
C13—C14—C15—C16	−1.0 (12)	C24—C25—C26—C21	1.7 (9)
Cl14—C14—C15—C16	−179.7 (6)	C22—C21—C26—C25	−1.4 (9)
C12—C11—C16—C15	0.2 (10)	C2—C21—C26—C25	176.9 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	1.96	2.818 (7)	166

C2—H2*A*···*Cg*1^{i}	0.99	2.96	3.498 (8)	115

Symmetry code: (i) *x*, *y*−1, *z*.

(IV) *N*-(4-Bromo-3-methylphenyl)-2-(2-chlorophenyl)acetamide

Crystal data

$C_{15}H_{13}BrClNO$
$M_r = 338.62$
Monoclinic, $P2_1/c$
$a = 11.8458$ (8) Å
$b = 4.7282$ (3) Å
$c = 25.0757$ (15) Å
$\beta = 98.133$ (5)°
$V = 1390.35$ (15) Å^3
$Z = 4$
$F(000) = 680$
$D_x = 1.618$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4745 reflections
$\theta = 3.3$–33.0°
$\mu = 3.14$ mm^{-1}
$T = 173$ K
Needle, colourless
0.38 × 0.12 × 0.08 mm

Data collection

Agilent Eos Gemini diffractometer
Radiation source: Enhance (Mo) X-ray Source
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min} = 0.373$, $T_{max} = 0.778$
10821 measured reflections
3201 independent reflections
2177 reflections with $I > 2\sigma(I)$
$R_{int} = 0.084$
$\theta_{max} = 27.6°$, $\theta_{min} = 3.3°$
$h = -15 \rightarrow 15$
$k = -5 \rightarrow 6$
$l = -30 \rightarrow 32$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.141$
$S = 1.08$
3201 reflections
173 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 0.2861P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.58$ e Å^{-3}
$\Delta\rho_{min} = -0.67$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2579 (3)	0.6288 (9)	0.29380 (16)	0.0230 (9)
O1	0.2592 (3)	0.8859 (6)	0.28824 (12)	0.0346 (8)
N1	0.2915 (3)	0.4470 (7)	0.25784 (13)	0.0235 (8)
H1	0.2877	0.2651	0.2648	0.028*
C2	0.2236 (4)	0.4897 (9)	0.34319 (17)	0.0305 (10)
H2A	0.2910	0.3969	0.3638	0.037*
H2B	0.1660	0.3417	0.3320	0.037*

C11	0.3328 (3)	0.5284 (8)	0.20926 (16)	0.0203 (9)
C12	0.2722 (4)	0.7259 (8)	0.17483 (17)	0.0243 (9)
H12	0.2036	0.8044	0.1839	0.029*
C13	0.3114 (4)	0.8082 (8)	0.12760 (17)	0.0234 (9)
C14	0.4118 (4)	0.6899 (9)	0.11661 (16)	0.0247 (9)
Br14	0.47195 (4)	0.79352 (12)	0.05281 (2)	0.0442 (2)
C15	0.4720 (4)	0.4935 (10)	0.14980 (17)	0.0301 (10)
H15	0.5409	0.4160	0.1409	0.036*
C16	0.4307 (4)	0.4104 (9)	0.19651 (17)	0.0272 (10)
H16	0.4704	0.2722	0.2195	0.033*
C17	0.2426 (4)	1.0184 (9)	0.09054 (18)	0.0318 (11)
H17A	0.2168	0.9282	0.0558	0.048*
H17B	0.2904	1.1822	0.0851	0.048*
H17C	0.1763	1.0805	0.1068	0.048*
C21	0.1750 (4)	0.7001 (8)	0.37901 (17)	0.0251 (9)
C22	0.0654 (4)	0.8118 (10)	0.36675 (18)	0.0313 (10)
Cl22	−0.01863 (11)	0.7074 (3)	0.30764 (5)	0.0498 (4)
C23	0.0216 (4)	1.0041 (10)	0.4003 (2)	0.0383 (12)
H23	−0.0539	1.0738	0.3914	0.046*
C24	0.0888 (5)	1.0927 (10)	0.4464 (2)	0.0405 (12)
H24	0.0598	1.2268	0.4693	0.049*
C25	0.1984 (4)	0.9884 (11)	0.4600 (2)	0.0408 (12)
H25	0.2444	1.0488	0.4921	0.049*
C26	0.2400 (4)	0.7939 (9)	0.42601 (18)	0.0326 (11)
H26	0.3153	0.7232	0.4353	0.039*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.025 (2)	0.021 (2)	0.023 (2)	−0.0002 (17)	0.0062 (16)	0.0026 (16)
O1	0.063 (2)	0.0094 (15)	0.0360 (19)	−0.0026 (14)	0.0208 (15)	0.0031 (12)
N1	0.037 (2)	0.0104 (18)	0.024 (2)	−0.0017 (14)	0.0070 (15)	0.0050 (13)
C2	0.042 (3)	0.023 (2)	0.029 (3)	0.006 (2)	0.015 (2)	0.0035 (18)
C11	0.025 (2)	0.013 (2)	0.022 (2)	−0.0036 (16)	0.0009 (16)	0.0006 (15)
C12	0.026 (2)	0.020 (2)	0.027 (2)	−0.0006 (17)	0.0046 (17)	0.0011 (16)
C13	0.029 (2)	0.015 (2)	0.026 (2)	−0.0026 (17)	0.0004 (17)	0.0012 (16)
C14	0.025 (2)	0.028 (2)	0.022 (2)	−0.0089 (18)	0.0053 (16)	−0.0027 (17)
Br14	0.0441 (3)	0.0629 (4)	0.0279 (3)	−0.0102 (3)	0.0128 (2)	0.0054 (2)
C15	0.025 (2)	0.037 (3)	0.029 (3)	−0.0005 (19)	0.0035 (18)	−0.0037 (19)
C16	0.024 (2)	0.024 (2)	0.033 (3)	0.0054 (18)	0.0050 (18)	0.0010 (18)
C17	0.041 (3)	0.023 (3)	0.031 (3)	0.001 (2)	0.002 (2)	0.0061 (18)
C21	0.033 (3)	0.018 (2)	0.026 (2)	0.0011 (18)	0.0109 (18)	0.0037 (17)
C22	0.035 (3)	0.032 (3)	0.027 (3)	−0.012 (2)	0.0063 (19)	0.0043 (19)
Cl22	0.0424 (8)	0.0640 (10)	0.0407 (8)	−0.0137 (6)	−0.0021 (6)	−0.0001 (6)
C23	0.037 (3)	0.035 (3)	0.046 (3)	0.003 (2)	0.016 (2)	0.006 (2)
C24	0.056 (3)	0.027 (3)	0.044 (3)	0.004 (2)	0.025 (2)	−0.003 (2)
C25	0.055 (3)	0.039 (3)	0.029 (3)	−0.002 (2)	0.009 (2)	−0.007 (2)
C26	0.039 (3)	0.031 (3)	0.029 (3)	0.002 (2)	0.007 (2)	0.0017 (19)

Geometric parameters (Å, º)

C1—O1	1.224 (5)	C15—H15	0.9500
C1—N1	1.346 (5)	C16—H16	0.9500
C1—C2	1.508 (5)	C17—H17A	0.9800
N1—C11	1.428 (5)	C17—H17B	0.9800
N1—H1	0.8800	C17—H17C	0.9800
C2—C21	1.508 (6)	C21—C26	1.387 (6)
C2—H2A	0.9900	C21—C22	1.395 (6)
C2—H2B	0.9900	C22—C23	1.388 (6)
C11—C16	1.365 (6)	C22—Cl22	1.736 (5)
C11—C12	1.399 (5)	C23—C24	1.374 (7)
C12—C13	1.387 (6)	C23—H23	0.9500
C12—H12	0.9500	C24—C25	1.385 (7)
C13—C14	1.377 (6)	C24—H24	0.9500
C13—C17	1.517 (5)	C25—C26	1.391 (6)
C14—C15	1.377 (6)	C25—H25	0.9500
C14—Br14	1.905 (4)	C26—H26	0.9500
C15—C16	1.388 (6)		
O1—C1—N1	123.3 (4)	C11—C16—C15	119.6 (4)
O1—C1—C2	122.4 (4)	C11—C16—H16	120.2
N1—C1—C2	114.3 (4)	C15—C16—H16	120.2
C1—N1—C11	124.7 (3)	C13—C17—H17A	109.5
C1—N1—H1	117.7	C13—C17—H17B	109.5
C11—N1—H1	117.7	H17A—C17—H17B	109.5
C1—C2—C21	111.8 (3)	C13—C17—H17C	109.5
C1—C2—H2A	109.3	H17A—C17—H17C	109.5
C21—C2—H2A	109.3	H17B—C17—H17C	109.5
C1—C2—H2B	109.3	C26—C21—C22	117.0 (4)
C21—C2—H2B	109.3	C26—C21—C2	120.3 (4)
H2A—C2—H2B	107.9	C22—C21—C2	122.7 (4)
C16—C11—C12	120.5 (4)	C23—C22—C21	122.0 (4)
C16—C11—N1	119.6 (4)	C23—C22—Cl22	119.0 (4)
C12—C11—N1	119.9 (4)	C21—C22—Cl22	118.9 (4)
C13—C12—C11	120.7 (4)	C24—C23—C22	119.3 (5)
C13—C12—H12	119.7	C24—C23—H23	120.4
C11—C12—H12	119.7	C22—C23—H23	120.4
C14—C13—C12	117.3 (4)	C23—C24—C25	120.6 (5)
C14—C13—C17	123.2 (4)	C23—C24—H24	119.7
C12—C13—C17	119.5 (4)	C25—C24—H24	119.7
C13—C14—C15	122.8 (4)	C24—C25—C26	119.1 (5)
C13—C14—Br14	120.0 (3)	C24—C25—H25	120.4
C15—C14—Br14	117.2 (3)	C26—C25—H25	120.4
C14—C15—C16	119.1 (4)	C21—C26—C25	122.0 (5)
C14—C15—H15	120.5	C21—C26—H26	119.0
C16—C15—H15	120.5	C25—C26—H26	119.0

O1—C1—N1—C11	0.3 (6)	C12—C11—C16—C15	1.9 (6)
C2—C1—N1—C11	−177.0 (4)	N1—C11—C16—C15	−178.8 (4)
O1—C1—C2—C21	8.9 (6)	C14—C15—C16—C11	−1.3 (7)
N1—C1—C2—C21	−173.8 (4)	C1—C2—C21—C26	−103.7 (5)
C1—N1—C11—C16	131.9 (4)	C1—C2—C21—C22	75.5 (5)
C1—N1—C11—C12	−48.7 (6)	C26—C21—C22—C23	−1.2 (6)
C16—C11—C12—C13	−0.9 (6)	C2—C21—C22—C23	179.6 (4)
N1—C11—C12—C13	179.7 (4)	C26—C21—C22—Cl22	178.6 (3)
C11—C12—C13—C14	−0.6 (6)	C2—C21—C22—Cl22	−0.5 (6)
C11—C12—C13—C17	178.8 (4)	C21—C22—C23—C24	1.4 (7)
C12—C13—C14—C15	1.1 (6)	Cl22—C22—C23—C24	−178.4 (4)
C17—C13—C14—C15	−178.2 (4)	C22—C23—C24—C25	−1.0 (7)
C12—C13—C14—Br14	−179.6 (3)	C23—C24—C25—C26	0.5 (7)
C17—C13—C14—Br14	1.1 (6)	C22—C21—C26—C25	0.6 (7)
C13—C14—C15—C16	−0.2 (7)	C2—C21—C26—C25	179.8 (4)
Br14—C14—C15—C16	−179.5 (3)	C24—C25—C26—C21	−0.3 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	1.93	2.802 (4)	170
C2—H2*B*···*Cg*1^{i}	0.99	2.99	3.552 (5)	117

Symmetry code: (i) *x*, *y*−1, *z*.