Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Six closely related 4,6-disubstituted 2-amino-5-formylpyrimidines: different ring conformations, polarized electronic structures, and hydrogen-bonded assembly in zero, one, two and three dimensions

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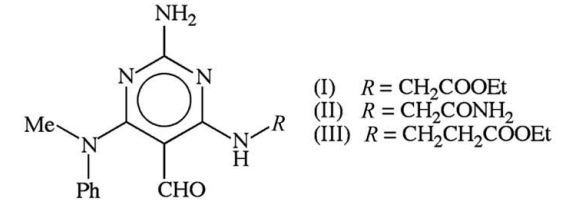
Received 20 November 2012
Accepted 17 December 2012
Online 8 January 2013

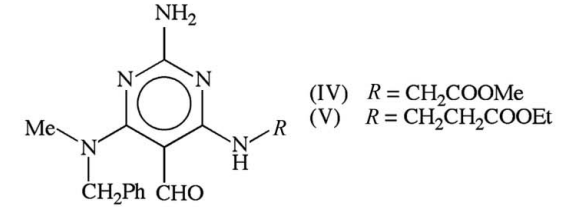
In each of ethyl *N*-{2-amino-5-formyl-6-[methyl(phenyl)amino]pyrimidin-4-yl}glycinate, $C_{16}H_{19}N_5O_3$, (I), *N*-{2-amino-5-formyl-6-[methyl(phenyl)amino]pyrimidin-4-yl}glycinamide, $C_{14}H_{16}N_6O_2$, (II), and ethyl 3-amino-*N*-{2-amino-5-formyl-6-[methyl(phenyl)amino]pyrimidin-4-yl}propionate, $C_{17}H_{21}N_5O_3$, (III), the pyrimidine ring is effectively planar, but in each of methyl *N*-{2-amino-6-[benzyl(methyl)amino]-5-formylpyrimidin-4-yl}glycinate, $C_{16}H_{19}N_5O_3$, (IV), ethyl 3-amino-*N*-{2-amino-6-[benzyl(methyl)amino]-5-formylpyrimidin-4-yl}propionate, $C_{18}H_{23}N_5O_3$, (V), and ethyl 3-amino-*N*-[2-amino-5-formyl-6-(piperidin-4-yl)pyrimidin-4-yl]propionate, $C_{15}H_{23}N_5O_3$, (VI), the pyrimidine ring is folded into a boat conformation. The bond lengths in each of (I)–(VI) provide evidence for significant polarization of the electronic structure. The molecules of (I) are linked by paired N—H···N hydrogen bonds to form isolated dimeric aggregates, and those of (III) are linked by a combination of N—H···N and N—H···O hydrogen bonds into a chain of edge-fused rings. In the structure of (IV), molecules are linked into sheets by means of two hydrogen bonds, both of N—H···O type, in the structure of (V) by three hydrogen bonds, two of N—H···N type and one of C—H···O type, and in the structure of (VI) by four hydrogen bonds, all of N—H···O type. Molecules of (II) are linked into a three-dimensional framework structure by a combination of three N—H···O hydrogen bonds and one C—H···O hydrogen bond.

Comment

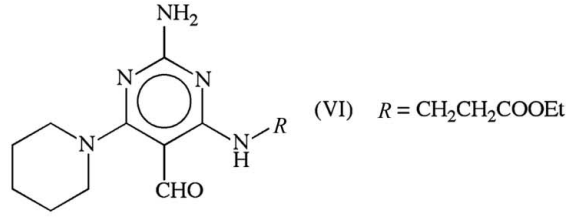
When heterocyclic species are covalently linked to biomolecules such as amino acids and peptides, carbohydrates, DNA or steroids, this type of combination can enhance the bioactivity of both components. For example, pyrimidine derivatives have been used in this way, particularly when linked to essential amino acids, in searches for new potentially bioactive agents, including anti-inflammatory agents (Bruno *et al.*, 1999), antimicrobials (Ghorab *et al.*, 2004), antidiabetic agents (Cantin *et al.*, 2006) and agents for the treatment of urinary tract disease (Murata *et al.*, 2004). Such combinations have also been investigated as potential intermediates for the synthesis of poly-fused pyrimidines of possible biological value (Min *et al.*, 2008). Here, we report the molecular and supramolecular structures of six compounds of this type, (I)–(VI) (Fig. 1 and Scheme), all having a simple amino substituent at position 6 of the pyrimidine ring, while position 4 of said ring carries, in each case, an amino substituent derived from a simple amino acid derivative. The present work is a development of an earlier study (Cobo *et al.*, 2008) which reported the structures of 12 N^6-substituted 2-amino-4-chloro-5-formylpyrimidines.



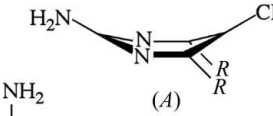
(I) $R = CH_2COOEt$
(II) $R = CH_2CONH_2$
(III) $R = CH_2CH_2COOEt$



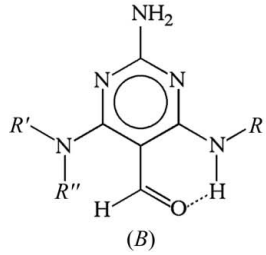
(IV) $R = CH_2COOMe$
(V) $R = CH_2CH_2COOEt$



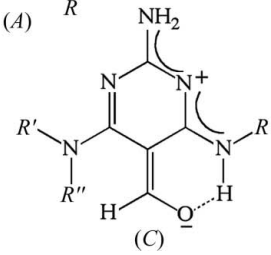
(VI) $R = CH_2CH_2COOEt$



(*A*)



(*B*)



(*C*)

Minor variations in one or other of the substituents at positions 4 and 6 in these compounds can lead to significant

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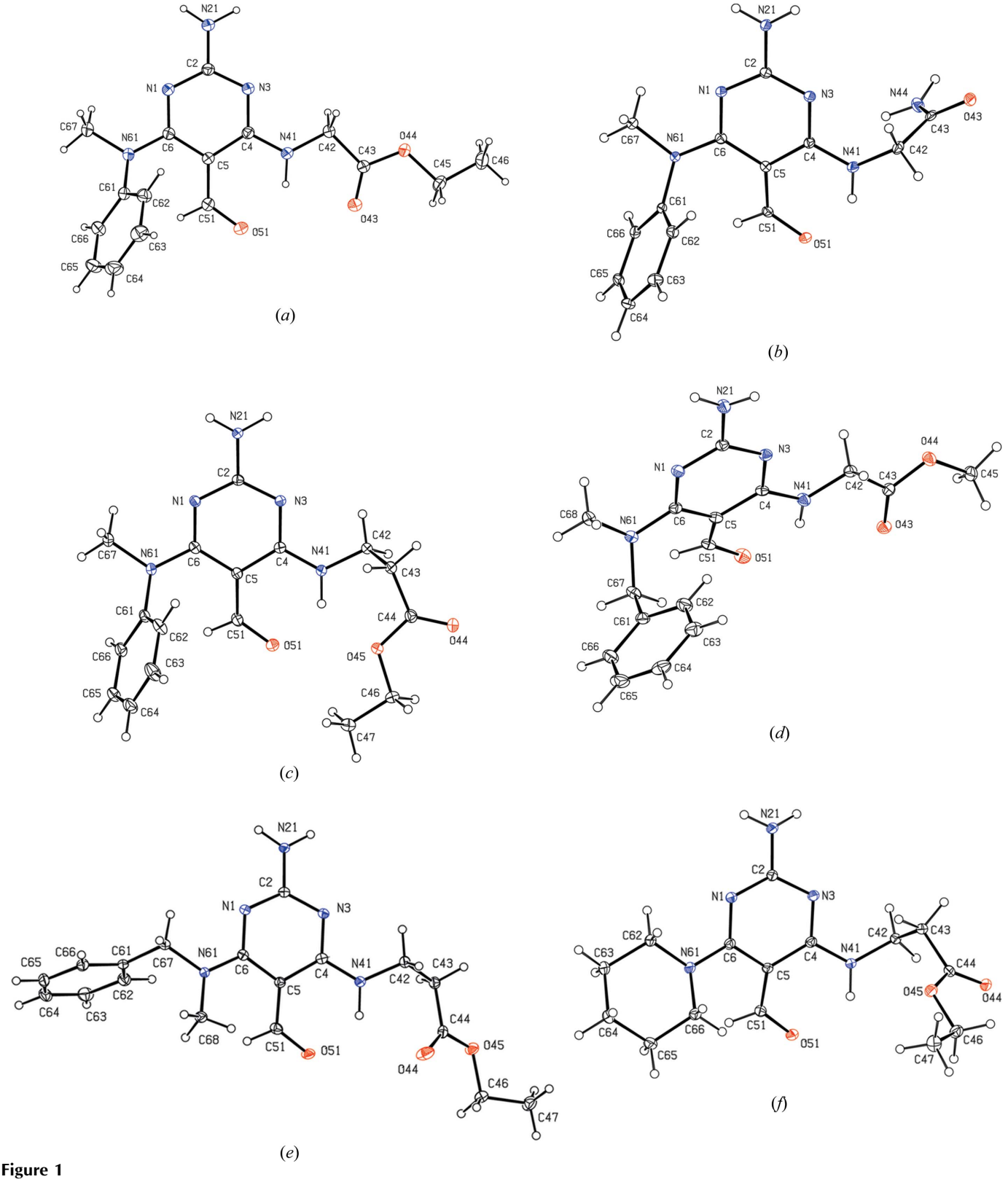

Figure 1
The molecular structures of compounds (I)–(VI), showing the atom-labelling schemes: (*a*) (I), (*b*) (II), (*c*) (III), (*d*) (IV), (*e*) (V) and (*f*) (VI). Displacement ellipsoids are drawn at the 20% probability level for (I) and at the 30% probability level for (II)–(VI).

differences, in both the molecular conformations and the hydrogen-bonded supramolecular assemblies. None of the molecules of (I)–(VI) exhibits any internal symmetry and they are all conformationally chiral, although all of them crystallize in centrosymmetric space groups. The reference molecules were selected so that all have the same sign for the torsion

angle C4—C5—C51—O51 (Table 1). In each structure, formyl atom O51 is involved in an intramolecular N—H···O hydrogen bond (Table 2), forming an *S*(6) motif (Bernstein *et al.*, 1995).

Compounds (I)–(III) (Fig. 1) all have an *N*-methyl-*N*-phenyl substituent at position 6 of the pyrimidine ring with slightly different substituents at position 4 (Fig. 1), *viz.* a glycinate ester and a glycinamide substituent in (I) and (II), respectively, and a 3-aminopropionate ester substituent in (III), and in each of (I)–(III) the pyrimidine ring is effectively planar. Compounds (IV) and (V) both have an *N*-benzyl-*N*-methyl substituent at position 6, with different amino acid ester substituents at position 4; the orientation of the 6-substituent is different, as indicated by the torsion angles C5—C6—N61—C67 and C5—C6—N61—C68 (Table 1 and Fig. 1). In addition, the pyrimidine ring in each of (IV)–(VI) is slightly distorted from planarity into a boat conformation, as indicated by the ring-puckering parameters (Cremer & Pople, 1975) for the atom sequence N1–C2–N3–C4–C5–C6 (Table 1). Thus, the ring-puckering parameters for compounds (IV)–(VI) are all very similar, and in each case the boat conformation has atoms C2 and C5 as the prow and stern of the boat, respectively, displaced to one side of the mean plane through the ring atoms, with atoms N1, N3, C4 and C6 all displaced to the opposite side of this plane, indicated schematically as (*A*) in the Scheme. Where three substituents are present at the 4-, 5- and 6-positions in pyrimidines, the ring is often found to be quite markedly nonplanar, leading to boat (Quesada *et al.*, 2004; Low *et al.*, 2007; Trilleras *et al.*, 2007; Cobo *et al.*, 2008), twist-boat (Melguizo *et al.*, 2003; Quesada *et al.*, 2003; Cobo *et al.*, 2008) or screw-boat (Low *et al.*, 2007) conformations, as well as a variety of intermediate forms (Cobo *et al.*, 2008). The conformations of (IV)–(VI) reported here are thus fully consistent with some of the examples reported earlier. However, even when the pyrimidine ring is effectively planar, as in (I)–(III), the ring substituent atoms are not always coplanar with the ring, with atom C51 always markedly displaced from the mean plane (Table 1).

While the glycinate ester side chains at position 4 in (I) and (IV) both adopt all-*transoid* extended-chain conformations, as demonstrated by the relevant torsion angles, which all lie within 10° of 180°, the corresponding aminopropionate substituents in (III), (V) and (VI) show a considerable variation in their conformations (Table 1 and Fig. 1). In particular, the values of the three torsion angles C4—N41—C42—C43, N41—C42—C43—C44 and C42—C43—C44—O45 show wide variations among these compounds. While it is tempting to associate these variations with the different patterns of hydrogen bonds involving this substituent in (III), (V) and (VI), such an approach cannot readily be reconciled with the similarity in the conformations of the 4-substituent in (I) and (IV), where the hydrogen bonds involving the 4-substituent are also different, with no involvement at all in (I), but participation of atom O43 in (IV) (Table 2).

There are some interesting patterns in the bond lengths in (I)–(VI) (Table 1) which suggest that the polarized form (*C*) (see Scheme) is a significant contributor to the overall electronic structure, in addition to the classical aromatic form (*B*). Within the formyl fragments, the C—O distance is, in every case, long for its type [reference mean = 1.192 Å and upper quartile = 1.197 Å; Allen *et al.* (1987, 2006)], while the C5—C51 bond between the formyl group and the pyrimidine ring is short for its type (reference mean = 1.470 Å and lower quartile = 1.463 Å). The N21—C2, C2—N3, N3—C4 and C4—N41 bond lengths (Fig. 1) are all very similar in each compound, despite the fact that the C2—N3 and N3—C4 bonds are formally of heteroaromatic type, while the exocyclic N21—C2 and C4—N41 bonds are formally single bonds. It may also be noted here that the N1—C2 bond is usually the longest of the ring N—C bonds, while the C6—N61 bond is consistently longer than the C4—N41 bond, and this may be associated with the fact that, in general, the substituents at N61 are usually displaced well away from the mean pyrimidine plane by a rotation about the C6—N61 bond. Moreover, the geometry at N61 is always slightly pyramidal, with a mean sum of the bond angles of 353.6 (2) Å, while atom N41 is always effectively planar.

The supramolecular assembly is dominated by N—H···N and N—H···O hydrogen bonds, with C—H···O hydrogen bonds also present in the structures of (II) and (V) and a C—H···N hydrogen bond present in the structure of (VI). C—H···O interactions involving C—H bonds in methyl groups, and those having *D*—H···*A* angles significantly less than 140°, have been discounted (*cf.* Wood *et al.*, 2009). However, N—H···π(arene) and C—H···π(arene) hydrogen bonds are absent, while the polarized pyrimidine rings are far from being aromatic. Despite the rather similar constitutions of (I)–(VI), the patterns of their hydrogen-bonded supramolecular assemblies vary widely, from simple dimeric units in (I), *via* chains and sheets, to a three-dimensional framework structure

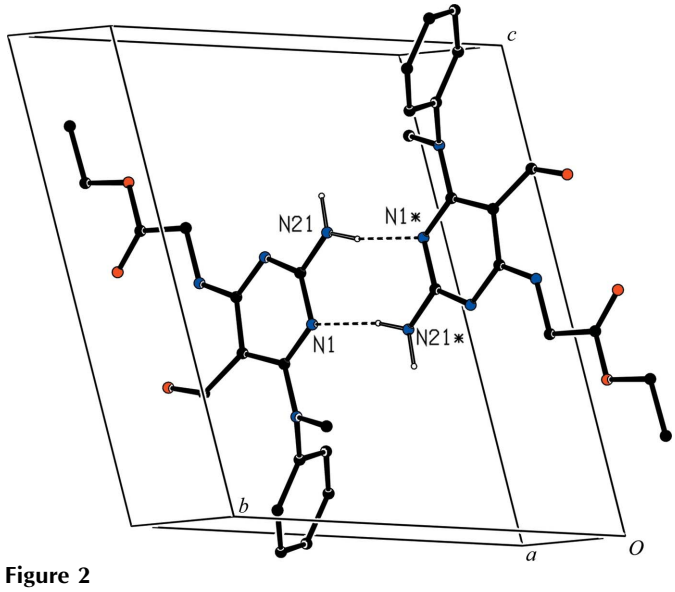

Figure 2
Part of the crystal structure of (I), showing the formation of a centrosymmetric hydrogen-bonded (dashed lines) $R_2^2(8)$ dimer. For the sake of clarity, H atoms other than those bonded to atom N21 have been omitted. Atoms marked with an asterisk (*) are at the symmetry position $(-x, -y + 1, -z + 1)$.

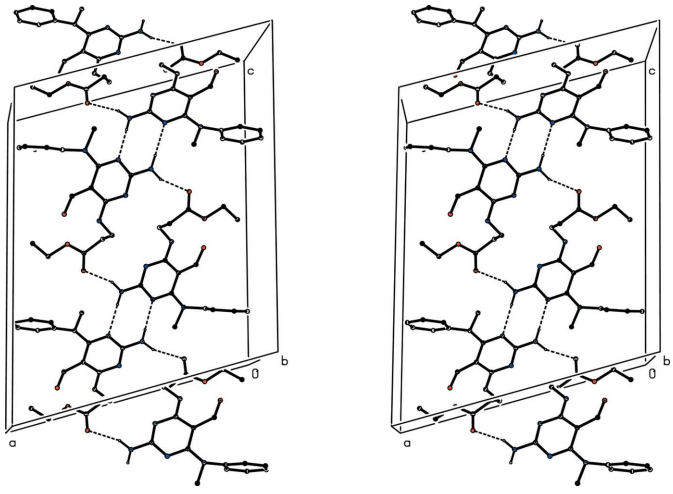

Figure 3
A stereoview of part of the crystal structure of (III), showing the formation of a hydrogen-bonded (dashed lines) chain of $R_2^2(8)$ and $R_2^2(20)$ rings along [001]. For the sake of clarity, H atoms other than those bonded to atom N21 have been omitted.

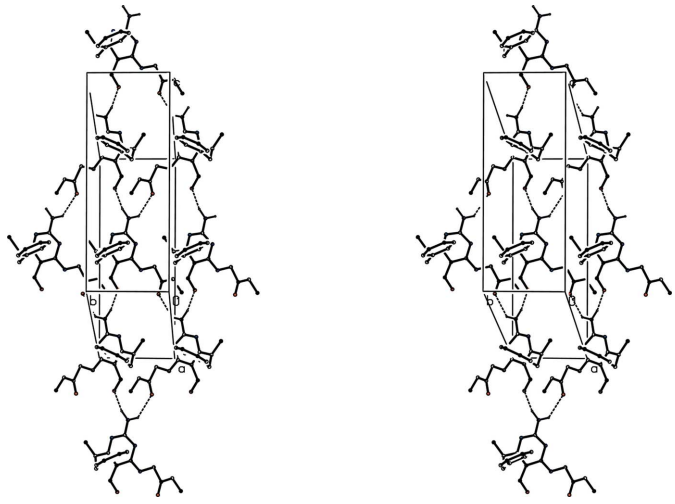

Figure 4
A stereoview of part of the crystal structure of (IV), showing the formation of a hydrogen-bonded (dashed lines) sheet of $R_4^4(28)$ rings lying parallel to (100). For the sake of clarity, H atoms other than those bonded to atom N21 have been omitted.

in (II). It is convenient to consider the hydrogen-bonded structures in order of increasing complexity.

In the structure of (I), there is only a single intermolecular hydrogen bond, of N—H···N type, and pairs of such bonds link inversion-related pairs of molecules into dimers characterized by a centrosymmetric $R_2^2(8)$ (Bernstein *et al.*, 1995) motif (Fig. 2).

The molecules of (III) are linked into a chain of edge-fused rings by a combination of N—H···N and N—H···O hydrogen bonds. A pair of molecules related by the twofold rotation axis along $(\frac{1}{2}, y, \frac{1}{4})$ are linked by symmetry-related N—H···N hydrogen bonds, using the same donor and acceptor as in (I) and forming an $R_2^2(8)$ ring, while a pair of molecules related by inversion are linked by symmetry-related N—H···O hydrogen bonds to form an $R_2^2(20)$ motif centred at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. The combination of these two motifs, propagated by rotation and inversion, generates a chain of edge-fused rings running parallel to the [001] direction, with $R_2^2(20)$ rings centred at $(\frac{1}{2}, \frac{1}{2}, \frac{n}{2})$, where n represents an integer, alternating with $R_2^2(8)$ rings lying across the twofold axes along $(\frac{1}{2}, y, \frac{1}{4} + \frac{n}{2})$, where n again represents an integer (Fig. 3).

Compounds (IV), (V) and (VI) all form sheets of increasing complexity and built using two, three and four hydrogen bonds, respectively (Table 2). There is no obvious correlation between the complexity of the supramolecular assemblies and the complexity, specifically the number of symmetry operators, of the space groups concerned, $P2_1/c$, $C2/c$ and $P\overline{1}$, respectively. In (IV), amino atom N21 in the molecule at (x, y, z) acts as hydrogen-bond donor, *via* atom H21*A*, to formyl atom O51 in the molecule at $(x, -y + \frac{3}{2}, z + \frac{1}{2})$, so forming a $C(9)$ chain running parallel to the [001] direction and built from molecules related by the 2_1 screw axis along $(0, \frac{3}{4}, z)$. This same atom, N21, also acts as hydrogen-bond donor, this time *via* atom H21*B*, to ester atom O43 in the molecule at $(x, -y + \frac{1}{2}, z + \frac{1}{2})$, forming a $C(9)$ chain, also parallel to [001] and containing molecules related by the 2_1 screw axis along $(0, \frac{1}{4}, z)$. The combination of these two chain motifs generates a sheet lying parallel to (100), in the form of a (4,4) net containing a single type of $R_4^4(28)$ ring (Fig. 4).

While the sheet in (IV) is built from two N—H···O hydrogen bonds, intermolecular hydrogen bonds of this type are absent from the structure of (V). Instead, the supramolecular assembly depends upon two hydrogen bonds of N—H···N type and one of C—H···O type (Table 2), and the formation of the sheet is most readily analysed in terms of two one-dimensional substructures (Ferguson *et al.*, 1998*a*,*b*; Gregson *et al.*, 2000). In the first substructure, the two N—H···N hydrogen bonds, acting in isolation, each forms a $C(4)$ chain running parallel to the [010] direction, and in combination they generate a chain of edge-fused rings containing molecules related by the 2_1 screw axis along $(\frac{3}{4}, y, \frac{3}{4})$ (Fig. 5). The C—H···O hydrogen bond links inversion-related pairs of molecules to form a centrosymmetric $R_2^2(22)$ motif. The molecule at (x, y, z) lies in the chain of edge-fused rings along

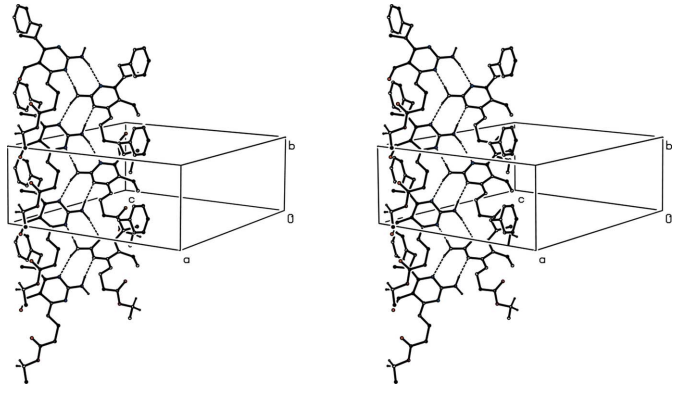

Figure 5
A stereoview of part of the crystal structure of (V), showing the formation of a hydrogen-bonded (dashed lines) chain of edge-fused $R_2^2(8)$ rings along [010]. For the sake of clarity, H atoms other than those bonded to atom N21 have been omitted.

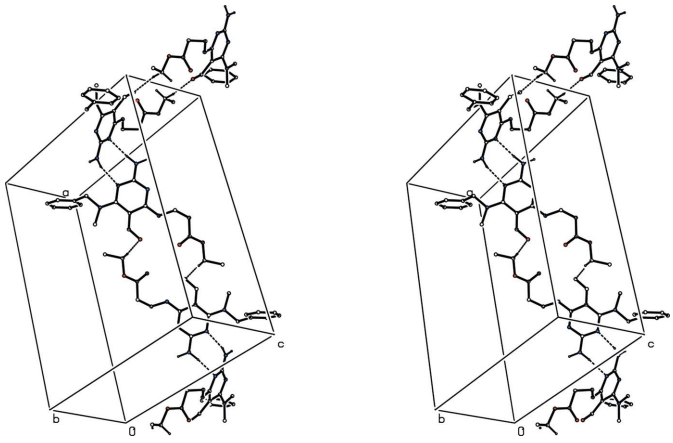

Figure 6
A stereoview of part of the crystal structure of (V), showing the formation of a hydrogen-bonded (dashed lines) chain of alternating $R_2^2(8)$ and $R_2^2(22)$ rings along [111]. For the sake of clarity, H atoms other than those bonded to atoms N21 and C46 have been omitted.

($\frac{3}{4}$, y, $\frac{3}{4}$), while that at ($-x+1$, $-y+1$, $-z+1$) forms part of a similar chain along ($\frac{1}{4}$, y, $\frac{1}{4}$). The combination of all three hydrogen bonds generates a chain of rings running parallel to the [111] direction in which $R_2^2(8)$ and $R_2^2(22)$ rings alternate (Fig. 6). The combination of the [101] and [111] substructural chains then generates a complex sheet lying parallel to (10$\overline{1}$).

Hydrogen bonds of N—H···N type are absent from the structure of (VI), where the sheet structure is generated by N—H···O hydrogen bonds (Table 2). As for (V), it is convenient to describe the formation of the sheet structure in (VI) in terms of two one-dimensional substructures. In one substructure, amino atom N21 acts as hydrogen-bond donor, *via* atoms H21*A* and H21*B*, to ester atoms O44 in the molecules at (x, $y+1$, z) and ($-x$, $-y+1$, $-z$), respectively, and these interactions generate a chain of edge-fused centrosymmetric rings running parallel to the [010] direction, within which $R_4^2(8)$ rings centred at (0, n, 0) alternate with $R_2^2(20)$ rings centred at (0, $\frac{1}{2}+n$, 0), where n represents an integer in both cases (Fig. 7). There is an intermolecular C—H···N contact in the structure, involving the α-CH_2 group of the carboxylate unit as donor. If this is regarded as structurally significant, its role is modestly to reinforce the chain along [010]. Amino atom N41 participates in a planar three-centre N—H···$(O)_2$ hydrogen bond, where the acceptors are two formyl O51 atoms at (x, y, z) and ($-x$, $-y+1$, $-z+1$) (Table 2), forming, respectively, $S(6)$ and $R_2^2(4)$ motifs. The combination of these motifs with the $R_2^2(20)$ motif produces a second substructure in the form of a chain of rings running parallel to the [001] direction, with $R_2^2(20)$ rings centred at (0, $\frac{1}{2}$, n) alternating with $R_2^2(4)$ rings centred at (0, $\frac{1}{2}$, $\frac{1}{2}+n$),

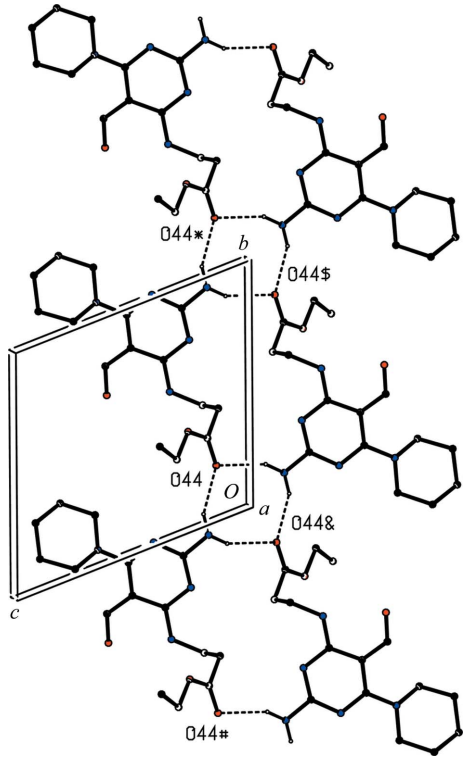

Figure 7
Part of the crystal structure of compound (VI), showing the formation of a hydrogen-bonded (dashed lines) chain of alternating $R_4^2(8)$ and $R_2^2(20)$ rings along [010]. For the sake of clarity, H atoms other than those bonded to atom N21 have been omitted. Atoms marked with an asterisk (*), a hash symbol (#), a dollar sign ($) or an ampersand (&) are at the symmetry positions (x, $y+1$, z), (x, $y-1$, z), ($-x$, $-y+1$, $-z$) and ($-x$, $-y$, $-z$), respectively.

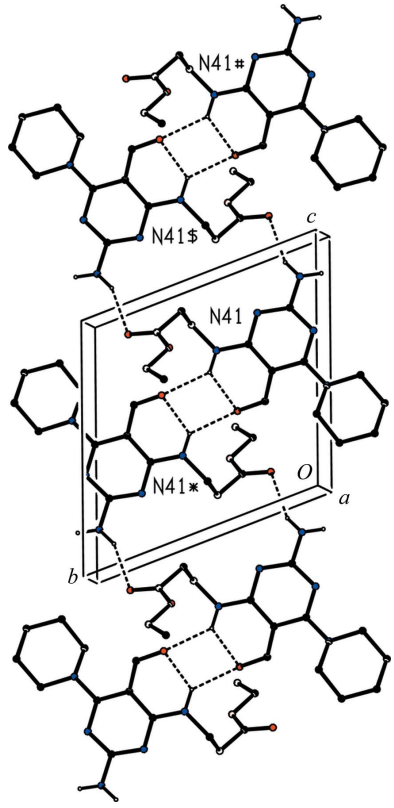

Figure 8
Part of the crystal structure of (VI), showing the formation of a hydrogen-bonded (dashed lines) chain of alternating $R_2^2(4)$ and $R_2^2(20)$ rings along [001]. For the sake of clarity, H atoms other than those bonded to atoms N21 and N41 have been omitted. Atoms marked with an asterisk (*), a hash symbol (#) or a dollar sign ($) are at the symmetry positions ($-x$, $-y+1$, $-z+1$), (x, y, $z+1$) and ($-x$, $-y+1$, $-z+2$), respectively.

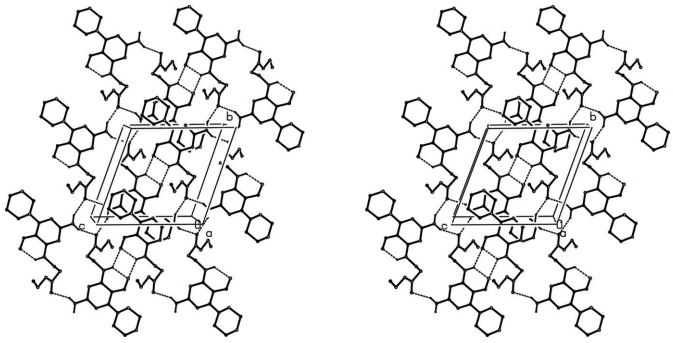

Figure 9
A stereoview of part of the crystal structure of (VI), showing the formation of a hydrogen-bonded (dashed lines) sheet lying parallel to (100). For the sake of clarity, H atoms other than those bonded to atoms N21 and N41 have been omitted.

where *n* represents an integer (Fig. 8). The combination of the substructures parallel to [010] and [001] generates a sheet lying parallel to (100) (Fig. 9).

Compound (II) is the only example amongst those discussed here in which the hydrogen-bonded supramolecular assembly is three-dimensional. The formation of this three-dimensional framework is most conveniently analysed in terms of the linking of sheets generated solely by N—H···O hydrogen bonds, and the formation of the sheet structure in turn is most readily analysed in terms of two substructures in the form of chains. In the simpler of the two chain motifs comprising the sheet, molecules related by translation are linked into a $C(9)$ chain running parallel to the [010] direction (Fig. 10). It is interesting to note that only one of the N—H bonds in the amide unit containing atom N21 participates in the hydrogen bonding.

The second chain motif in (II) involves the two N—H bonds of the amide unit containing atom N44. This atom, in the reference molecule at (x, y, z), acts as hydrogen-bond donor, *via* atom H44*A*, to formyl atom O51 at ($-x+1$, y, $-z+\frac{1}{2}$), so forming an $R_2^2(18)$ ring containing two molecules related by the twofold rotation axis along ($\frac{1}{2}$, y, $\frac{1}{4}$). Atom N44 at (x, y, z) also acts as donor, this time *via* atom H44*B*, to amide atom O43 at ($-x+\frac{3}{2}$, $-y+\frac{1}{2}$, $-z+1$), so forming an $R_2^2(8)$ ring containing two molecules related by inversion across ($\frac{3}{4}$, $\frac{1}{4}$, $\frac{1}{2}$). The combination of these two motifs generates a chain of edge-fused rings running parallel to the [101] direction, with $R_2^2(8)$ rings centred at ($\frac{1}{4}+\frac{n}{2}$, $\frac{1}{4}$, $\frac{n}{2}$) alternating with $R_2^2(8)$ rings lying across the twofold rotation axes along ($\frac{n}{2}$, y, $-\frac{1}{4}+\frac{n}{2}$), where n represents an integer in each case (Fig. 11).

The combination of the simple chain along [010] and the chain of rings along [101] generates a sheet lying parallel to ($10\overline{1}$). Two sheets of this type, related to one another by inversion, pass through each unit cell, and adjacent sheets are linked by the third substructural motif, so generating a three-dimensional framework structure. Aryl atom C62 in the molecule at (x, y, z) acts as hydrogen-bond donor to amide atom O43 at ($-x+1$, $-y+1$, $-z+1$), so forming a centrosymmetric $R_2^2(22)$ ring (Fig. 12) in which the two component molecules lie in different ($10\overline{1}$) sheets. Propagation of this interaction by the space-group symmetry operators serves to link all of the sheets into a single continuous structure.

In summary, we have shown that the hydrogen-bonded assembly of six very closely related pyrimidine derivatives varies widely, emcompassing a simple dimeric unit, chains, sheets and a three-dimensional framework structure.

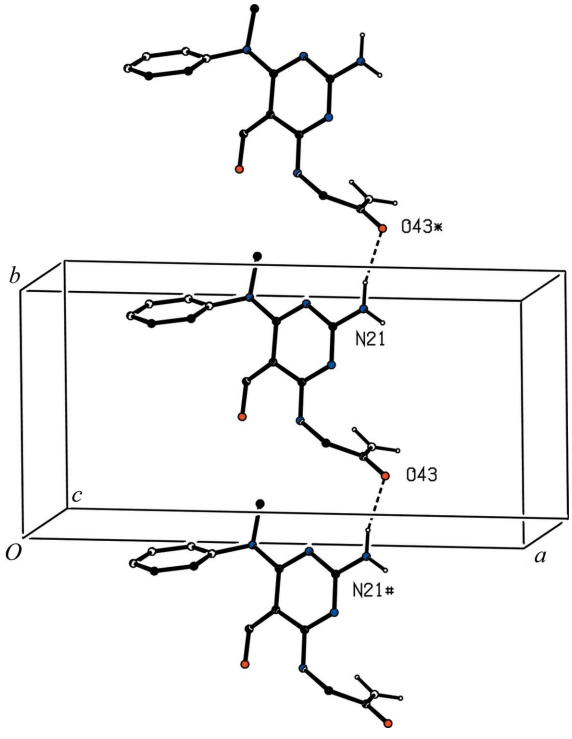

Figure 10
Part of the crystal structure of (II), showing the formation of a hydrogen-bonded (dashed lines) $C(9)$ chain along [010]. For the sake of clarity, H atoms other than those bonded to atoms N21 and N44 have been omitted. Atoms marked with an asterisk (*) or a hash symbol (#) are at the symmetry positions (x, $y+1$, z) and (x, $y-1$, z), respectively.

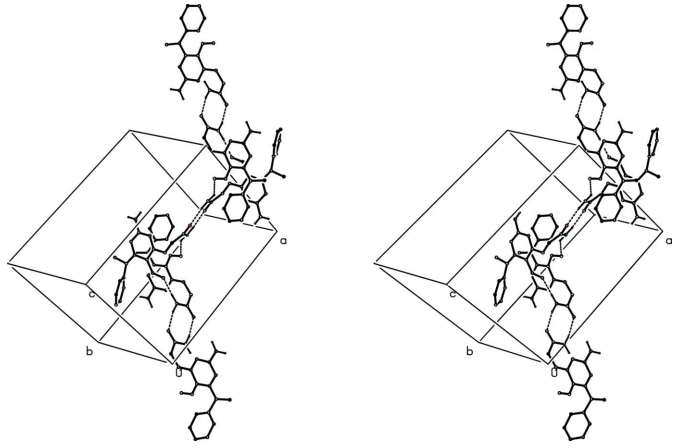

Figure 11
A stereoview of part of the crystal structure of (II), showing the formation of a hydrogen-bonded (dashed lines) chain of alternating $R_2^2(8)$ and $R_2^2(18)$ rings along [101]. For the sake of clarity, H atoms other than those bonded to atoms N21 and N44 have been omitted.

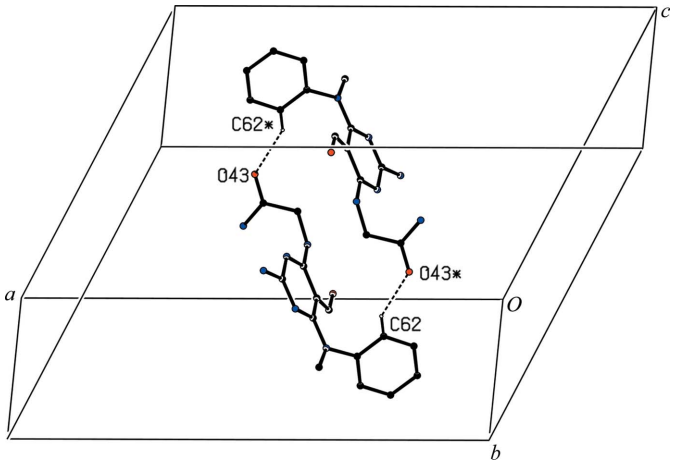

Figure 12
Part of the crystal structure of (II), showing the formation of the centrosymmetric $R_2^2(22)$ motif which links the $(10\overline{1})$ sheets. Hydrogen bonds are shown as dashed lines. For the sake of clarity, H atoms not involved in the motif shown have been omitted. Atoms marked with an asterisk (*) are at the symmetry position $(-x+1, -y+1, -z+1)$.

Experimental

For the synthesis of the esters (I) and (III)–(VI), the appropriate amino ester hydrochloride (1.3 mmol) and anhydrous potassium carbonate (6.5 mmol) were added to a suspension of the appropriate N^4-substituted 2,4-diamino-6-chloropyrimidine-5-carbaldehyde in dry acetonitrile (10 ml). The mixtures were then heated under reflux until thin-layer chromatography (TLC) indicated that the starting pyrimidine had all been consumed. The mixtures were then cooled to ambient temperature and the solvent was removed under reduced pressure. The resulting products were then purified by flash chromatography on silica gel using dichloromethane/acetone mixtures (95:5 to 90:10 *v*/*v*) as eluent. Finally, crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation of solutions in methanol at ambient temperature and in air.

Compound (I), from 2-amino-4-chloro-6-[methyl(phenyl)amino]-pyrimidine-5-carbaldehyde and glycine ethyl ester hydrochloride. Reaction time 24 h, yield 83%, pale yellow, m.p. 394 K (decomposition). MS (EI, 70 eV) *m*/*z* (%): 329 (M^+, 92), 328 (100), 312 (51), 200 (41), 254 (68), 238 (43), 226 (66). Analysis found: C 58.1, H 5.9, N 20.9%; $C_{16}H_{19}N_5O_3$ requires: C 58.3, H 5.8, N 21.3%.

Compound (III), from 2-amino-4-chloro-6-[methyl(phenyl)amino]-pyrimidine-5-carbaldehyde and β-alanine ethyl ester hydrochloride. Reaction time 20 h, yield 78%, colourless, m.p. >433 K (decomposition). MS (EI, 70 eV) *m*/*z* (%): 3443 (M^+, 79), 342 (100), 254 (62), 214 (40). Analysis found: C 59.5, H 5.9, N 19.9%; $C_{17}H_{21}N_5O_3$ requires: C 59.5, H 6.2, N 20.4%.

Compound (IV), from 2-amino-6-[benzyl(methyl)amino]-4-chloro-pyrimidine-5-carbaldehyde and glycine ethyl ester hydrochloride. Reaction time 4 d, yield 87%, colourless, m.p. 388 K (decomposition). MS (EI, 70 eV) *m*/*z* (%): 329 (M^+, 77), 313 (20), 312 (100), 300 (31), 270 (21), 259 (29), 120 (73), 91 (65).

Compound (V), from 2-amino-6-[benzyl(methyl)amino]-4-chloro-pyrimidine-5-carbaldehyde and β-alanine ethyl ester hydrochloride. Reaction time 24 h, yield 88%, colourless, m.p. 388 K (decomposition). MS (EI, 70 eV) *m*/*z* (%): 357 (M^+, 53), 340 (72), 328 (20), 312 (26), 270 (13), 266 (26), 252 (31), 192 (82), 91 (100). Analysis found: C 60.7, H 6.2, N 19.2%; $C_{18}H_{23}N_5O_3$ requires: C 60.5, H 6.5, N 19.6%.

Compound (VI), from 2-amino-4-chloro-6-(piperidin-1-yl)pyrimidine-5-carbaldehyde and β-alanine ethyl ester hydrochloride. Reaction time 21 h, yield 99%, colourless, m.p. 378 K. MS (EI, 70 eV) *m*/*z* (%): 321 (M^+, 42), 304 (100), 276 (25), 230 (18), 216 (26). Analysis found: C 55.7, H 7.4, N 21.7%; $C_{15}H_{23}N_5O_3$ requires: C 56.1, H 7.2, N 21.8%.

For the synthesis of (II), a sample of (I) (0.3 mmol) was added to a methanol ammonia solution (5 ml of 7 M), and this mixture was then held at 313 K for 6 h. The solvent and the excess ammonia were removed under reduced pressure at ambient temperature and the product was crystallized from methanol [yield 75%, colourless, m.p. >413 K (decomposition)]. MS (EI, 70 eV) *m*/*z* (%): 300 (M^+, 65), 299 (100), 283 (17), 256 (92), 254 (67), 238 (44), 226 (56), 212 (34), 200 (22), 106 (20). HRMS found: 300.1331; $C_{14}H_{16}N_6O_2$ requires 300.1335.

Compound (I)

Crystal data

$C_{16}H_{19}N_5O_3$
M_r = 329.36
Triclinic, $P\overline{1}$
a = 7.3990 (5) Å
b = 9.609 (3) Å
c = 12.449 (3) Å
α = 73.30 (2)°
β = 82.680 (14)°
γ = 72.693 (13)°
V = 808.5 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.41 × 0.25 × 0.22 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.885, T_{max} = 0.936
18365 measured reflections
3006 independent reflections
2054 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.120
S = 1.02
3006 reflections
220 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Compound (II)

Crystal data

$C_{14}H_{16}N_6O_2$
M_r = 300.33
Monoclinic, $C2/c$
a = 20.045 (4) Å
b = 8.6868 (7) Å
c = 17.990 (3) Å
β = 114.064 (11)°
V = 2860.3 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 120 K
0.32 × 0.20 × 0.11 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.969, T_{max} = 0.989
32858 measured reflections
2657 independent reflections
1993 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.119
S = 1.12
2657 reflections
200 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °) for compounds (I)–(VI).

(i) Bond lengths

Parameter	(I)	(II)	(III)	(IV)	(V)	(VI)
N1—C2	1.353 (2)	1.350 (3)	1.361 (2)	1.353 (3)	1.346 (2)	1.353 (3)
C2—N3	1.340 (2)	1.352 (3)	1.341 (2)	1.342 (3)	1.346 (2)	1.344 (2)
N3—C4	1.335 (2)	1.336 (3)	1.346 (2)	1.339 (3)	1.346 (2)	1.335 (3)
C4—C5	1.430 (2)	1.436 (3)	1.433 (2)	1.436 (3)	1.441 (3)	1.434 (3)
C5—C6	1.418 (2)	1.438 (3)	1.428 (2)	1.429 (3)	1.430 (3)	1.421 (3)
C6—N1	1.335 (2)	1.336 (3)	1.339 (2)	1.331 (3)	1.351 (2)	1.324 (3)
C2—N21	1.342 (2)	1.337 (3)	1.340 (2)	1.340 (3)	1.345 (2)	1.336 (3)
C4—N41	1.336 (2)	1.352 (3)	1.343 (2)	1.334 (3)	1.343 (2)	1.339 (3)
C5—C51	1.426 (3)	1.426 (3)	1.432 (3)	1.420 (3)	1.426 (3)	1.409 (3)
C51—O51	1.232 (2)	1.247 (3)	1.239 (2)	1.239 (3)	1.241 (2)	1.234 (2)
C6—N61	1.380 (2)	1.371 (3)	1.381 (2)	1.381 (3)	1.359 (2)	1.378 (3)

(ii) Torsion angles

N3—C4—N41—C42	−4.8 (2)	7.0 (3)	3.2 (3)	−2.4 (3)	11.0 (3)	−0.9 (3)
C4—N41—C42—C43	−196.15 (17)	−88.6 (3)	114.35 (19)	−178.5 (2)	−138.69 (18)	78.2 (2)
N41—C42—C43—C44			74.4 (2)		−63.1 (2)	81.2 (2)
N41—C42—C43—N44		1.3 (3)				
N41—C42—C43—O44	−172.71 (17)			170.47 (19)		
C42—C43—C44—O45			−68.3 (2)		−174.63 (16)	−109.4 (2)
C43—C44—O45—C46			179.43 (16)		−177.40 (16)	−179.55 (17)
C44—O45—C46—C47			−174.16 (16)		−147.25 (18)	171.90 (18)
C42—C43—O44—C45	178.29 (17)			177.2 (2)		
C43—O44—C45—C46	170.04 (19)					
C4—C5—C51—O51	13.1 (3)	8.3 (4)	13.2 (3)	15.3 (4)	11.5 (3)	14.9 (3)
C5—C6—N61—C61	42.6 (3)	35.4 (3)	39.4 (2)			
C5—C6—N61—C62						−174.97 (18)
C5—C6—N61—C66						43.4 (3)
C5—C6—N61—C67	−161.27 (18)	−175.8 (2)	−171.57 (16)	46.0 (3)	−170.05 (17)	
C5—C6—C61—C68				−169.3 (2)	22.5 (3)	

(iii) Substituent displacement from mean pyrimidine plane

Compound	N21	N41	C51	O51	N61
(I)	0.077 (2)	−0.015 (2)	0.319 (2)	0.334 (2)	−0.071 (2)
(II)	0.132 (2)	−0.035 (2)	0.321 (2)	0.391 (2)	−0.101 (2)
(III)	0.106 (2)	−0.162 (2)	0.353 (2)	0.331 (2)	−0.084 (2)
(IV)	0.161 (2)	−0.037 (2)	0.444 (3)	0.487 (2)	−0.190 (2)
(V)	0.300 (2)	−0.172 (2)	0.493 (2)	0.548 (2)	−0.256 (2)
(VI)	0.245 (2)	−0.104 (2)	0.564 (2)	0.670 (2)	−0.251 (2)

(iv) Ring-puckering parameters

Compound	Q	θ	φ
(IV)	0.100 (3)	97.0 (17)	76.9 (14)
(V)	0.156 (3)	98.5 (7)	59.8 (7)
(VI)	0.149 (2)	96.9 (8)	71.8 (8)
Idealized boat		90.0	60*n*

Compound (III)

Crystal data

$C_{17}H_{21}N_5O_3$
M_r = 343.39
Monoclinic, $C2/c$
a = 16.707 (6) Å
b = 10.218 (2) Å
c = 20.733 (5) Å
β = 105.929 (19)°
V = 3403.5 (16) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 120 K
0.29 × 0.22 × 0.10 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.973, T_{max} = 0.991
21914 measured reflections
3160 independent reflections
2239 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.095
S = 1.09
3160 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Compound (IV)

Crystal data

$C_{16}H_{19}N_5O_3$
M_r = 329.36
Monoclinic, $P2_1/c$
a = 15.636 (4) Å
b = 6.5674 (18) Å
c = 17.336 (5) Å
β = 113.440 (18)°
V = 1633.3 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 120 K
0.29 × 0.27 × 0.15 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer	21188 measured reflections 3013 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	2209 reflections with $I > 2\sigma(I)$
T_{min} = 0.973, T_{max} = 0.986	R_{int} = 0.072

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059	219 parameters
$wR(F^2)$ = 0.165	H-atom parameters constrained
S = 1.09	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
3013 reflections	$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Compound (V)

Crystal data

$C_{18}H_{23}N_5O_3$	V = 3505.0 (8) Å^3
M_r = 357.41	Z = 8
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 24.8226 (5) Å	μ = 0.10 mm^{-1}
b = 7.1379 (14) Å	T = 120 K
c = 20.601 (2) Å	0.26 × 0.21 × 0.14 mm
β = 106.213 (8)°	

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer	22384 measured reflections 3269 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	2276 reflections with $I > 2\sigma(I)$
T_{min} = 0.976, T_{max} = 0.987	R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045	237 parameters
$wR(F^2)$ = 0.104	H-atom parameters constrained
S = 1.06	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
3269 reflections	$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Compound (VI)

Crystal data

$C_{15}H_{23}N_5O_3$	γ = 103.10 (3)°
M_r = 321.38	V = 781.2 (8) Å^3
Triclinic, $P\overline{1}$	Z = 2
a = 8.040 (4) Å	Mo $K\alpha$ radiation
b = 10.391 (3) Å	μ = 0.10 mm^{-1}
c = 10.458 (8) Å	T = 120 K
α = 109.16 (3)°	0.41 × 0.25 × 0.22 mm
β = 98.19 (5)°	

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer	17622 measured reflections 3227 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	2384 reflections with $I > 2\sigma(I)$
T_{min} = 0.885, T_{max} = 0.936	R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051	209 parameters
$wR(F^2)$ = 0.134	H-atom parameters constrained
S = 1.05	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
3227 reflections	$\Delta\rho_{min}$ = −0.32 e Å^{-3}

All H atoms were located in difference maps. C-bound H atoms were subsequently treated as riding atoms in geometrically idealized positions, with C—H = 0.93–0.99 Å and U_{iso}(H) = kU_{eq}(C), where k = 1.5 for the methyl groups, which were permitted to rotate but not to tilt, and 1.2 for all other C-bound H atoms. N-bound H atoms were permitted to ride at the positions deduced from the difference maps, with U_{iso}(H) = 1.2U_{eq}(N), giving N—H distances in the range 0.77–1.01 Å (see Table 2).

Table 2
Hydrogen bonds and short intramolecular contacts (Å, °) for compounds (I)–(VI).

Compound	D—H···A	D—H	H···A	D···A	D—H···A
(I)	N21—H21A···N1^{i}	0.92	2.22	3.125 (2)	167
	N41—H41···O51	0.94	1.90	2.675 (2)	138
(II)	N21—H21A···O43^{ii}	0.94	2.02	2.933 (2)	166
	N41—H41···O51	0.90	1.98	2.689 (2)	135
	N44—H44A···O51^{iii}	0.95	2.14	2.949 (2)	143
	N44—H44B···O43^{iv}	0.98	2.05	3.006 (3)	164
	C62—H62···O43^{v}	0.95	2.45	3.280 (3)	146
(III)	N21—H21A···N1^{iii}	0.90	2.14	3.027 (2)	169
	N21—H21B···O44^{v}	0.97	2.14	3.054 (2)	158
	N41—H41···O51	0.96	1.95	2.683 (2)	131
(IV)	N21—H21A···O51^{vi}	1.00	1.89	2.860 (3)	163
	N21—H21B···O43^{vii}	0.89	2.38	3.085 (3)	136
	N41—H41···O51	0.96	1.92	2.682 (3)	135
(V)	N21—H21A···N3^{viii}	0.96	2.07	3.008 (2)	168
	N21—H21B···N1^{ix}	0.95	2.30	3.199 (2)	158
	N41—H41···O44	1.01	2.27	2.891 (2)	119
	N41—H41···O51	1.01	1.92	2.666 (2)	128
	C46—H46A···O51^{x}	0.99	2.54	3.528 (3)	172
(VI)	N21—H21A···O44^{ii}	0.88	2.15	2.951 (3)	150
	N21—H21B···O44^{xi}	0.89	2.20	3.036 (3)	156
	N41—H41···O51	0.94	2.05	2.700 (3)	125
	N41—H41···O51^{i}	0.94	2.21	2.909 (3)	131
	C43—H43A···N3^{xi}	0.99	2.55	3.524 (4)	169

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x, y+1, z$; (iii) $-x+1, y, -z+\frac{1}{2}$; (iv) $-x+\frac{3}{2}, -y+\frac{1}{2}, -z+1$; (v) $-x+1, -y+1, -z+1$; (vi) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (vii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (viii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (ix) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (x) $-x+1, -y, -z+1$; (xi) $-x, -y+1, -z$.

For all compounds, data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2000); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* and *PLATON*.

The authors thank the Centro de Instrumentación Científico-Técnica of the Universidad de Jaén and the staff for the data collection. JC thanks the Consejería de Innovación, Ciencia y Empresa (Junta de Andalucía, Spain), the Universidad de Jaén (UJA) and the Ministerio de Ciencia e Innovación (project No. SAF2008-04685-C02-02) for financial support. AP, LMA and AFY thank the Colombian Institute for Science and Research (COLCIENCIAS, grant No. 1102-521-28229). AFY and LMA both also thank the Asociación Universitaria Iberoamericana de Postgrado (AUIP) for supporting a research stage at UJA.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: YF3022). Services for accessing these data are described at the back of the journal.

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supplementary materials

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Six closely related 4,6-disubstituted 2-amino-5-formylpyrimidines: different ring conformations, polarized electronic structures, and hydrogen-bonded assembly in zero, one, two and three dimensions

Lina M. Acosta, Andrés F. Yepes, Alirio Palma, Justo Cobo and Christopher Glidewell

(I) Ethyl *N*-{2-amino-5-formyl-6-[methyl(phenyl)amino]pyrimidin-4-yl}glycinate

Crystal data

$C_{16}H_{19}N_5O_3$
M_r = 329.36
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.3990 (5) Å
b = 9.609 (3) Å
c = 12.449 (3) Å
α = 73.30 (2)°
β = 82.680 (14)°
γ = 72.693 (13)°
V = 808.5 (3) Å^3
Z = 2
$F(000)$ = 348
D_x = 1.353 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3718 reflections
θ = 3.2–27.5°
μ = 0.10 mm^{-1}
T = 293 K
Block, pale yellow
0.41 × 0.25 × 0.22 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
Radiation source: Bruker Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.885, T_{max} = 0.936
18365 measured reflections
3006 independent reflections
2054 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 25.5°, θ_{min} = 3.2°
h = −8→8
k = −11→11
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.120
S = 1.02
3006 reflections
220 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
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.2215P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.033 (4)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.1832 (2)	0.62253 (17)	0.41032 (12)	0.0370 (4)
C2	0.2237 (2)	0.6088 (2)	0.51649 (15)	0.0358 (4)
N3	0.3581 (2)	0.65340 (17)	0.54930 (12)	0.0372 (4)
C4	0.4570 (2)	0.7269 (2)	0.46709 (15)	0.0343 (4)
C5	0.4235 (2)	0.7561 (2)	0.35103 (15)	0.0348 (4)
C6	0.2866 (2)	0.6925 (2)	0.32890 (14)	0.0341 (4)
N21	0.1191 (2)	0.5411 (2)	0.59954 (13)	0.0488 (5)
H21A	0.0412	0.4884	0.5872	0.059*
H21B	0.1525	0.5227	0.6757	0.059*
N41	0.5891 (2)	0.77684 (18)	0.49610 (13)	0.0415 (4)
H41	0.6471	0.8364	0.4363	0.050*
C42	0.6239 (3)	0.7672 (2)	0.60966 (15)	0.0414 (5)
H42A	0.6666	0.6623	0.6520	0.050*
H42B	0.5087	0.8157	0.6465	0.050*
C43	0.7738 (3)	0.8457 (2)	0.60362 (16)	0.0417 (5)
O43	0.8323 (2)	0.9156 (2)	0.51776 (13)	0.0728 (5)
O44	0.83342 (19)	0.82899 (16)	0.70415 (11)	0.0464 (4)
C45	0.9843 (3)	0.8998 (3)	0.70299 (19)	0.0534 (6)
H45A	0.9497	1.0036	0.6575	0.064*
H45B	1.1011	0.8458	0.6708	0.064*
C46	1.0116 (4)	0.8957 (3)	0.8196 (2)	0.0657 (7)
H46A	1.0490	0.7926	0.8636	0.099*
H46B	0.8951	0.9484	0.8511	0.099*
H46C	1.1086	0.9435	0.8198	0.099*
C51	0.5014 (3)	0.8607 (2)	0.26646 (16)	0.0421 (5)
H51	0.4535	0.8904	0.1954	0.050*
O51	0.6259 (2)	0.91568 (17)	0.27831 (11)	0.0533 (4)
N61	0.2488 (2)	0.70546 (19)	0.22015 (12)	0.0406 (4)
C61	0.3994 (3)	0.6844 (2)	0.13638 (15)	0.0387 (5)
C62	0.5608 (3)	0.5669 (2)	0.16096 (17)	0.0474 (5)
H62	0.5737	0.5000	0.2322	0.057*
C63	0.7041 (3)	0.5488 (3)	0.0788 (2)	0.0614 (6)
H63	0.8151	0.4711	0.0958	0.074*
C64	0.6842 (4)	0.6443 (3)	−0.0276 (2)	0.0664 (7)
H64	0.7807	0.6305	−0.0825	0.080*
C65	0.5227 (4)	0.7593 (3)	−0.05232 (18)	0.0615 (6)
H65	0.5089	0.8240	−0.1243	0.074*
C66	0.3798 (3)	0.7799 (2)	0.02895 (16)	0.0502 (5)
H66	0.2696	0.8584	0.0116	0.060*
C67	0.0719 (3)	0.6819 (3)	0.19802 (18)	0.0557 (6)
H67A	−0.0287	0.7235	0.2462	0.084*
H67B	0.0864	0.5756	0.2123	0.084*
H67C	0.0422	0.7311	0.1210	0.084*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0371 (9)	0.0447 (9)	0.0343 (9)	−0.0186 (7)	0.0011 (7)	−0.0121 (7)
C2	0.0368 (10)	0.0391 (11)	0.0340 (10)	−0.0141 (9)	0.0028 (8)	−0.0115 (8)
N3	0.0398 (9)	0.0449 (9)	0.0325 (8)	−0.0206 (7)	0.0019 (7)	−0.0108 (7)
C4	0.0341 (10)	0.0363 (10)	0.0352 (10)	−0.0123 (8)	0.0004 (8)	−0.0119 (8)
C5	0.0347 (10)	0.0391 (11)	0.0332 (10)	−0.0147 (8)	−0.0005 (8)	−0.0093 (8)
C6	0.0330 (10)	0.0370 (10)	0.0329 (10)	−0.0103 (8)	−0.0014 (8)	−0.0093 (8)
N21	0.0562 (11)	0.0683 (12)	0.0347 (9)	−0.0392 (9)	0.0040 (8)	−0.0130 (8)
N41	0.0466 (9)	0.0544 (11)	0.0330 (9)	−0.0302 (8)	0.0009 (7)	−0.0104 (7)
C42	0.0466 (11)	0.0520 (12)	0.0326 (10)	−0.0234 (10)	−0.0010 (8)	−0.0118 (9)
C43	0.0468 (11)	0.0502 (12)	0.0346 (11)	−0.0245 (10)	0.0006 (9)	−0.0108 (9)
O43	0.0944 (12)	0.1037 (14)	0.0418 (9)	−0.0740 (11)	−0.0048 (8)	−0.0027 (9)
O44	0.0491 (8)	0.0653 (9)	0.0375 (8)	−0.0324 (7)	−0.0011 (6)	−0.0161 (7)
C45	0.0486 (12)	0.0679 (15)	0.0591 (14)	−0.0320 (11)	−0.0013 (10)	−0.0242 (11)
C46	0.0748 (16)	0.0708 (16)	0.0639 (15)	−0.0337 (13)	−0.0236 (13)	−0.0136 (13)
C51	0.0453 (11)	0.0471 (12)	0.0382 (11)	−0.0205 (10)	−0.0031 (9)	−0.0094 (9)
O51	0.0593 (9)	0.0638 (10)	0.0450 (8)	−0.0386 (8)	−0.0019 (7)	−0.0046 (7)
N61	0.0369 (9)	0.0580 (11)	0.0320 (8)	−0.0202 (8)	−0.0030 (7)	−0.0115 (7)
C61	0.0444 (11)	0.0453 (11)	0.0331 (10)	−0.0212 (9)	−0.0015 (8)	−0.0113 (9)
C62	0.0532 (13)	0.0459 (12)	0.0433 (12)	−0.0176 (10)	−0.0015 (10)	−0.0084 (9)
C63	0.0535 (14)	0.0606 (15)	0.0703 (16)	−0.0134 (12)	0.0068 (12)	−0.0243 (13)
C64	0.0729 (17)	0.0821 (19)	0.0557 (15)	−0.0365 (15)	0.0245 (13)	−0.0319 (14)
C65	0.0825 (18)	0.0749 (17)	0.0341 (12)	−0.0394 (15)	0.0075 (11)	−0.0109 (11)
C66	0.0589 (13)	0.0549 (13)	0.0368 (11)	−0.0195 (11)	−0.0059 (10)	−0.0065 (10)
C67	0.0478 (13)	0.0859 (17)	0.0412 (12)	−0.0326 (12)	−0.0075 (9)	−0.0116 (11)

Geometric parameters (Å, º)

N1—C6	1.335 (2)	C45—H45B	0.9700
N1—C2	1.353 (2)	C46—H46A	0.9600
C2—N3	1.340 (2)	C46—H46B	0.9600
C2—N21	1.342 (2)	C46—H46C	0.9600
N3—C4	1.335 (2)	C51—O51	1.232 (2)
C4—N41	1.336 (2)	C51—H51	0.9300
C4—C5	1.430 (2)	N61—C61	1.436 (2)
C5—C6	1.418 (2)	N61—C67	1.464 (2)
C5—C51	1.426 (3)	C61—C62	1.374 (3)
C6—N61	1.380 (2)	C61—C66	1.385 (3)
N21—H21A	0.9242	C62—C63	1.384 (3)
N21—H21B	0.9636	C62—H62	0.9300
N41—C42	1.441 (2)	C63—C64	1.375 (3)
N41—H41	0.9409	C63—H63	0.9300
C42—C43	1.500 (3)	C64—C65	1.362 (3)
C42—H42A	0.9700	C64—H64	0.9300
C42—H42B	0.9700	C65—C66	1.378 (3)
C43—O43	1.193 (2)	C65—H65	0.9300
C43—O44	1.330 (2)	C66—H66	0.9300
O44—C45	1.467 (2)	C67—H67A	0.9600

C45—C46	1.479 (3)	C67—H67B	0.9600
C45—H45A	0.9700	C67—H67C	0.9600
C6—N1—C2	115.75 (15)	C45—C46—H46A	109.5
N3—C2—N21	115.54 (16)	C45—C46—H46B	109.5
N3—C2—N1	127.77 (16)	H46A—C46—H46B	109.5
N21—C2—N1	116.68 (16)	C45—C46—H46C	109.5
C4—N3—C2	115.82 (15)	H46A—C46—H46C	109.5
N3—C4—N41	117.83 (16)	H46B—C46—H46C	109.5
N3—C4—C5	122.50 (16)	O51—C51—C5	126.41 (18)
N41—C4—C5	119.66 (16)	O51—C51—H51	116.8
C6—C5—C51	122.78 (17)	C5—C51—H51	116.8
C6—C5—C4	115.27 (16)	C6—N61—C61	120.97 (15)
C51—C5—C4	121.27 (16)	C6—N61—C67	119.49 (15)
N1—C6—N61	116.45 (16)	C61—N61—C67	115.42 (15)
N1—C6—C5	122.59 (16)	C62—C61—C66	119.58 (19)
N61—C6—C5	120.92 (16)	C62—C61—N61	120.45 (17)
C2—N21—H21A	122.3	C66—C61—N61	119.93 (18)
C2—N21—H21B	118.0	C61—C62—C63	119.4 (2)
H21A—N21—H21B	117.4	C61—C62—H62	120.3
C4—N41—C42	124.86 (15)	C63—C62—H62	120.3
C4—N41—H41	115.3	C64—C63—C62	120.7 (2)
C42—N41—H41	119.0	C64—C63—H63	119.6
N41—C42—C43	107.29 (15)	C62—C63—H63	119.6
N41—C42—H42A	110.3	C65—C64—C63	119.7 (2)
C43—C42—H42A	110.3	C65—C64—H64	120.1
N41—C42—H42B	110.3	C63—C64—H64	120.1
C43—C42—H42B	110.3	C64—C65—C66	120.2 (2)
H42A—C42—H42B	108.5	C64—C65—H65	119.9
O43—C43—O44	124.00 (18)	C66—C65—H65	119.9
O43—C43—C42	123.37 (18)	C65—C66—C61	120.3 (2)
O44—C43—C42	112.62 (15)	C65—C66—H66	119.9
C43—O44—C45	114.96 (15)	C61—C66—H66	119.9
O44—C45—C46	108.72 (17)	N61—C67—H67A	109.5
O44—C45—H45A	109.9	N61—C67—H67B	109.5
C46—C45—H45A	109.9	H67A—C67—H67B	109.5
O44—C45—H45B	109.9	N61—C67—H67C	109.5
C46—C45—H45B	109.9	H67A—C67—H67C	109.5
H45A—C45—H45B	108.3	H67B—C67—H67C	109.5
C6—N1—C2—N3	−1.9 (3)	O43—C43—O44—C45	−1.9 (3)
C6—N1—C2—N21	178.89 (16)	C42—C43—O44—C45	178.29 (17)
N21—C2—N3—C4	−177.11 (16)	C43—O44—C45—C46	170.04 (19)
N1—C2—N3—C4	3.7 (3)	C6—C5—C51—O51	−176.82 (19)
C2—N3—C4—N41	178.29 (16)	C4—C5—C51—O51	13.1 (3)
C2—N3—C4—C5	−0.3 (3)	N1—C6—N61—C61	−139.74 (18)
N3—C4—C5—C6	−4.1 (3)	C5—C6—N61—C61	42.6 (3)
N41—C4—C5—C6	177.27 (16)	N1—C6—N61—C67	16.4 (3)
N3—C4—C5—C51	166.67 (17)	C5—C6—N61—C67	−161.27 (18)

N41—C4—C5—C51	−11.9 (3)	C6—N61—C61—C62	43.8 (3)
C2—N1—C6—N61	179.10 (16)	C67—N61—C61—C62	−113.3 (2)
C2—N1—C6—C5	−3.3 (3)	C6—N61—C61—C66	−138.31 (19)
C51—C5—C6—N1	−164.61 (18)	C67—N61—C61—C66	64.7 (2)
C4—C5—C6—N1	6.1 (3)	C66—C61—C62—C63	2.1 (3)
C51—C5—C6—N61	12.9 (3)	N61—C61—C62—C63	180.00 (19)
C4—C5—C6—N61	−176.44 (16)	C61—C62—C63—C64	−1.8 (3)
N3—C4—N41—C42	−4.8 (3)	C62—C63—C64—C65	0.8 (4)
C5—C4—N41—C42	173.87 (18)	C63—C64—C65—C66	0.1 (4)
C4—N41—C42—C43	−176.15 (17)	C64—C65—C66—C61	0.2 (3)
N41—C42—C43—O43	7.4 (3)	C62—C61—C66—C65	−1.3 (3)
N41—C42—C43—O44	−172.71 (17)	N61—C61—C66—C65	−179.20 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21—H21*A*···N1^{i}	0.92	2.22	3.125 (2)	167
N41—H41···O51	0.94	1.90	2.675 (2)	138

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

(II) *N*-{2-Amino-5-formyl-6-[methyl(phenyl)amino]pyrimidin-4-yl}glycinamide

Crystal data

$C_{14}H_{16}N_6O_2$
M_r = 300.33
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 20.045 (4) Å
b = 8.6868 (7) Å
c = 17.990 (3) Å
β = 114.064 (11)°
V = 2860.3 (8) Å^3
Z = 8
F(000) = 1264
D_x = 1.395 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3290 reflections
θ = 2.6–27.5°
μ = 0.10 mm^{-1}
T = 120 K
Plate, colourless
0.32 × 0.20 × 0.11 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
Radiation source: Bruker Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.969, T_{max} = 0.989
32858 measured reflections
2657 independent reflections
1993 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 25.5°, θ_{min} = 2.6°
h = −24→24
k = −10→10
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.119
S = 1.12
2657 reflections
200 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
$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 5.1608P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.53486 (10)	0.9198 (2)	0.40896 (11)	0.0177 (4)
C2	0.58234 (12)	0.8233 (2)	0.46413 (13)	0.0176 (5)
N3	0.57839 (10)	0.6681 (2)	0.46616 (11)	0.0191 (4)
C4	0.52481 (12)	0.6035 (2)	0.40211 (13)	0.0161 (5)
C5	0.47362 (11)	0.6906 (2)	0.33536 (13)	0.0157 (5)
C6	0.48010 (11)	0.8548 (2)	0.34637 (12)	0.0157 (5)
N21	0.63877 (11)	0.8895 (2)	0.52450 (11)	0.0264 (5)
H21A	0.6428	0.9964	0.5215	0.032*
H21B	0.6728	0.8302	0.5639	0.032*
N41	0.52083 (10)	0.4481 (2)	0.40089 (11)	0.0199 (4)
H41	0.4833	0.4064	0.3586	0.024*
C42	0.56561 (12)	0.3514 (3)	0.46820 (13)	0.0200 (5)
H42A	0.5371	0.2578	0.4674	0.024*
H42B	0.5742	0.4071	0.5193	0.024*
C43	0.63942 (12)	0.3004 (2)	0.47167 (13)	0.0179 (5)
O43	0.67776 (9)	0.21582 (17)	0.52914 (9)	0.0228 (4)
N44	0.66162 (11)	0.3466 (2)	0.41535 (11)	0.0240 (5)
H44A	0.6306	0.4195	0.3782	0.029*
H44B	0.7127	0.3321	0.4232	0.029*
C51	0.42654 (11)	0.6197 (2)	0.26089 (13)	0.0163 (5)
H51	0.3990	0.6859	0.2171	0.020*
O51	0.41838 (8)	0.47834 (17)	0.24825 (9)	0.0208 (4)
N61	0.43222 (10)	0.9555 (2)	0.29196 (11)	0.0171 (4)
C61	0.35514 (12)	0.9229 (2)	0.24847 (13)	0.0161 (5)
C62	0.31485 (12)	0.8653 (3)	0.28957 (13)	0.0199 (5)
H62	0.3384	0.8384	0.3455	0.024*
C63	0.23939 (13)	0.8474 (3)	0.24764 (14)	0.0246 (5)
H63	0.2114	0.8079	0.2752	0.030*
C64	0.20517 (13)	0.8868 (3)	0.16633 (14)	0.0243 (5)
H64	0.1537	0.8767	0.1384	0.029*
C65	0.24613 (12)	0.9412 (3)	0.12547 (14)	0.0228 (5)
H65	0.2226	0.9658	0.0692	0.027*
C66	0.32116 (12)	0.9600 (2)	0.16621 (13)	0.0186 (5)
H66	0.3490	0.9978	0.1382	0.022*
C67	0.44708 (12)	1.1210 (2)	0.30632 (14)	0.0219 (5)
H67A	0.4990	1.1405	0.3208	0.033*
H67B	0.4344	1.1546	0.3509	0.033*
H67C	0.4177	1.1783	0.2568	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0172 (10)	0.0147 (9)	0.0164 (9)	−0.0011 (7)	0.0021 (8)	−0.0015 (7)

C2	0.0183 (12)	0.0169 (12)	0.0136 (11)	−0.0004 (9)	0.0023 (9)	−0.0003 (9)
N3	0.0186 (10)	0.0167 (10)	0.0156 (9)	−0.0009 (8)	0.0003 (8)	−0.0004 (8)
C4	0.0179 (11)	0.0140 (11)	0.0146 (11)	−0.0002 (9)	0.0047 (9)	−0.0017 (8)
C5	0.0143 (11)	0.0154 (11)	0.0160 (11)	0.0006 (9)	0.0047 (9)	0.0003 (9)
C6	0.0166 (11)	0.0167 (11)	0.0135 (11)	−0.0001 (9)	0.0059 (9)	−0.0013 (9)
N21	0.0270 (11)	0.0141 (10)	0.0209 (10)	−0.0020 (8)	−0.0080 (9)	0.0008 (8)
N41	0.0207 (10)	0.0155 (10)	0.0166 (9)	−0.0029 (8)	0.0006 (8)	−0.0008 (8)
C42	0.0274 (13)	0.0134 (11)	0.0162 (11)	−0.0022 (9)	0.0059 (10)	0.0015 (9)
C43	0.0227 (12)	0.0112 (11)	0.0146 (11)	−0.0046 (9)	0.0023 (9)	−0.0025 (9)
O43	0.0245 (9)	0.0186 (8)	0.0184 (8)	0.0004 (7)	0.0017 (7)	0.0024 (7)
N44	0.0239 (11)	0.0256 (11)	0.0187 (10)	0.0048 (9)	0.0047 (8)	0.0043 (8)
C51	0.0127 (11)	0.0172 (12)	0.0177 (11)	0.0017 (9)	0.0048 (9)	−0.0011 (9)
O51	0.0193 (8)	0.0163 (8)	0.0209 (8)	−0.0025 (7)	0.0022 (7)	−0.0052 (6)
N61	0.0156 (9)	0.0118 (9)	0.0185 (9)	−0.0005 (7)	0.0015 (8)	−0.0002 (7)
C61	0.0148 (11)	0.0116 (11)	0.0178 (11)	0.0014 (8)	0.0025 (9)	−0.0023 (8)
C62	0.0213 (12)	0.0195 (12)	0.0161 (11)	0.0016 (9)	0.0047 (9)	−0.0007 (9)
C63	0.0221 (13)	0.0290 (13)	0.0243 (12)	−0.0034 (10)	0.0111 (10)	−0.0029 (10)
C64	0.0151 (12)	0.0244 (13)	0.0260 (13)	−0.0009 (10)	0.0007 (10)	−0.0044 (10)
C65	0.0229 (13)	0.0188 (12)	0.0163 (11)	0.0034 (10)	−0.0027 (9)	0.0005 (9)
C66	0.0205 (12)	0.0142 (11)	0.0185 (11)	0.0012 (9)	0.0052 (9)	0.0020 (9)
C67	0.0197 (12)	0.0146 (12)	0.0244 (12)	−0.0013 (9)	0.0019 (10)	0.0006 (9)

Geometric parameters (Å, º)

N1—C6	1.336 (3)	N44—H44B	0.9820
N1—C2	1.350 (3)	C51—O51	1.247 (3)
C2—N21	1.337 (3)	C51—H51	0.9500
C2—N3	1.352 (3)	N61—C61	1.447 (3)
N3—C4	1.336 (3)	N61—C67	1.469 (3)
C4—N41	1.352 (3)	C61—C66	1.391 (3)
C4—C5	1.436 (3)	C61—C62	1.391 (3)
C5—C51	1.426 (3)	C62—C63	1.397 (3)
C5—C6	1.438 (3)	C62—H62	0.9500
C6—N61	1.371 (3)	C63—C64	1.382 (3)
N21—H21A	0.9359	C63—H63	0.9500
N21—H21B	0.9156	C64—C65	1.390 (3)
N41—C42	1.446 (3)	C64—H64	0.9500
N41—H41	0.8995	C65—C66	1.388 (3)
C42—C43	1.521 (3)	C65—H65	0.9500
C42—H42A	0.9900	C66—H66	0.9500
C42—H42B	0.9900	C67—H67A	0.9800
C43—O43	1.246 (3)	C67—H67B	0.9800
C43—N44	1.324 (3)	C67—H67C	0.9800
N44—H44A	0.9463		
C6—N1—C2	116.60 (18)	H44A—N44—H44B	122.3
N21—C2—N1	116.09 (19)	O51—C51—C5	125.7 (2)
N21—C2—N3	116.49 (19)	O51—C51—H51	117.1
N1—C2—N3	127.4 (2)	C5—C51—H51	117.1
C4—N3—C2	115.49 (18)	C6—N61—C61	122.89 (18)

N3—C4—N41	117.01 (19)	C6—N61—C67	117.80 (17)
N3—C4—C5	123.3 (2)	C61—N61—C67	112.46 (17)
N41—C4—C5	119.69 (19)	C66—C61—C62	120.7 (2)
C51—C5—C4	122.08 (19)	C66—C61—N61	118.8 (2)
C51—C5—C6	123.08 (19)	C62—C61—N61	120.42 (19)
C4—C5—C6	114.43 (19)	C61—C62—C63	119.2 (2)
N1—C6—N61	115.29 (19)	C61—C62—H62	120.4
N1—C6—C5	122.18 (19)	C63—C62—H62	120.4
N61—C6—C5	122.49 (19)	C64—C63—C62	120.3 (2)
C2—N21—H21A	116.4	C64—C63—H63	119.8
C2—N21—H21B	120.2	C62—C63—H63	119.8
H21A—N21—H21B	123.2	C63—C64—C65	119.9 (2)
C4—N41—C42	123.65 (19)	C63—C64—H64	120.0
C4—N41—H41	116.1	C65—C64—H64	120.0
C42—N41—H41	119.6	C66—C65—C64	120.5 (2)
N41—C42—C43	117.69 (19)	C66—C65—H65	119.8
N41—C42—H42A	107.9	C64—C65—H65	119.8
C43—C42—H42A	107.9	C65—C66—C61	119.3 (2)
N41—C42—H42B	107.9	C65—C66—H66	120.3
C43—C42—H42B	107.9	C61—C66—H66	120.3
H42A—C42—H42B	107.2	N61—C67—H67A	109.5
O43—C43—N44	121.9 (2)	N61—C67—H67B	109.5
O43—C43—C42	117.8 (2)	H67A—C67—H67B	109.5
N44—C43—C42	120.34 (19)	N61—C67—H67C	109.5
C43—N44—H44A	114.4	H67A—C67—H67C	109.5
C43—N44—H44B	120.4	H67B—C67—H67C	109.5

C6—N1—C2—N21	177.1 (2)	N41—C42—C43—N44	1.3 (3)
C6—N1—C2—N3	−4.5 (3)	C4—C5—C51—O51	8.3 (4)
N21—C2—N3—C4	−175.1 (2)	C6—C5—C51—O51	−179.4 (2)
N1—C2—N3—C4	6.4 (3)	N1—C6—N61—C61	−146.9 (2)
C2—N3—C4—N41	177.8 (2)	C5—C6—N61—C61	35.4 (3)
C2—N3—C4—C5	−0.8 (3)	N1—C6—N61—C67	1.9 (3)
N3—C4—C5—C51	167.3 (2)	C5—C6—N61—C67	−175.8 (2)
N41—C4—C5—C51	−11.3 (3)	C6—N61—C61—C66	−137.5 (2)
N3—C4—C5—C6	−5.7 (3)	C67—N61—C61—C66	72.2 (3)
N41—C4—C5—C6	175.8 (2)	C6—N61—C61—C62	46.9 (3)
C2—N1—C6—N61	179.15 (19)	C67—N61—C61—C62	−103.4 (2)
C2—N1—C6—C5	−3.2 (3)	C66—C61—C62—C63	−1.1 (3)
C51—C5—C6—N1	−165.2 (2)	N61—C61—C62—C63	174.5 (2)
C4—C5—C6—N1	7.7 (3)	C61—C62—C63—C64	−0.1 (3)
C51—C5—C6—N61	12.4 (3)	C62—C63—C64—C65	1.5 (4)
C4—C5—C6—N61	−174.8 (2)	C63—C64—C65—C66	−1.6 (4)
N3—C4—N41—C42	7.0 (3)	C64—C65—C66—C61	0.4 (3)
C5—C4—N41—C42	−174.3 (2)	C62—C61—C66—C65	1.0 (3)
C4—N41—C42—C43	−88.6 (3)	N61—C61—C66—C65	−174.65 (19)
N41—C42—C43—O43	−179.29 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21—H21*A*···O43^{i}	0.94	2.02	2.933 (2)	166
N41—H41···O51	0.90	1.98	2.689 (2)	135
N44—H44*A*···O51^{ii}	0.95	2.14	2.949 (2)	143
N44—H44*B*···O43^{iii}	0.98	2.05	3.006 (3)	164
C62—H62···O43^{iv}	0.95	2.45	3.280 (3)	146

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+1, *y*, −*z*+1/2; (iii) −*x*+3/2, −*y*+1/2, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1.

(III) Ethyl 3-amino-*N*-{2-amino-5-formyl-6-[methyl(phenyl)amino]pyrimidin- 4-yl}propionate

Crystal data

$C_{17}H_{21}N_5O_3$
M_r = 343.39
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 16.707 (6) Å
b = 10.218 (2) Å
c = 20.733 (5) Å
β = 105.929 (19)°
V = 3403.5 (16) Å^3
Z = 8
F(000) = 1456
D_x = 1.340 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3916 reflections
θ = 2.7–27.5°
μ = 0.10 mm^{-1}
T = 120 K
Plate, colourless
0.29 × 0.22 × 0.10 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
Radiation source: Bruker Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.973, T_{max} = 0.991
21914 measured reflections
3160 independent reflections
2239 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
θ_{max} = 25.5°, θ_{min} = 2.7°
h = −20→20
k = −12→12
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.095
S = 1.09
3160 reflections
228 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
$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 2.178P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.40872 (10)	0.17214 (14)	0.28821 (7)	0.0177 (3)
C2	0.46275 (11)	0.23317 (17)	0.34084 (8)	0.0168 (4)
N3	0.44497 (9)	0.28871 (14)	0.39387 (7)	0.0171 (3)
C4	0.36591 (11)	0.27637 (17)	0.39697 (8)	0.0163 (4)

C5	0.30520 (11)	0.20093 (17)	0.34921 (9)	0.0174 (4)
C6	0.33077 (12)	0.15698 (17)	0.29255 (9)	0.0177 (4)
N21	0.54146 (9)	0.24174 (15)	0.33734 (7)	0.0222 (4)
H21A	0.5558	0.2094	0.3016	0.027*
H21B	0.5819	0.2860	0.3731	0.027*
N41	0.34415 (10)	0.33671 (15)	0.44718 (7)	0.0200 (4)
H41	0.2882	0.3264	0.4506	0.024*
C42	0.39948 (12)	0.42037 (18)	0.49688 (9)	0.0219 (4)
H42A	0.4561	0.4159	0.4908	0.026*
H42B	0.4024	0.3869	0.5423	0.026*
C43	0.37086 (12)	0.56410 (18)	0.49202 (9)	0.0238 (5)
H43A	0.4176	0.6195	0.5174	0.029*
H43B	0.3565	0.5919	0.4445	0.029*
C44	0.29701 (12)	0.58623 (18)	0.51876 (9)	0.0224 (4)
O44	0.29875 (9)	0.64666 (14)	0.56953 (7)	0.0312 (4)
O45	0.22837 (8)	0.52993 (13)	0.48012 (6)	0.0233 (3)
C46	0.15224 (12)	0.5431 (2)	0.50101 (10)	0.0268 (5)
H46A	0.1341	0.6357	0.4983	0.032*
H46B	0.1612	0.5124	0.5477	0.032*
C47	0.08790 (13)	0.4597 (2)	0.45338 (10)	0.0309 (5)
H47A	0.0789	0.4926	0.4075	0.046*
H47B	0.0355	0.4633	0.4659	0.046*
H47C	0.1075	0.3690	0.4557	0.046*
C51	0.22888 (12)	0.16081 (18)	0.36199 (9)	0.0223 (4)
H51	0.1971	0.0960	0.3332	0.027*
O51	0.20072 (8)	0.20319 (13)	0.40731 (6)	0.0281 (3)
N61	0.27576 (10)	0.09496 (14)	0.23933 (7)	0.0198 (4)
C67	0.30784 (13)	0.0352 (2)	0.18652 (9)	0.0259 (5)
H67A	0.3126	0.1025	0.1541	0.039*
H67B	0.2695	−0.0333	0.1636	0.039*
H67C	0.3627	−0.0032	0.2069	0.039*
C61	0.19051 (12)	0.13782 (18)	0.21516 (9)	0.0208 (4)
C62	0.17252 (13)	0.2689 (2)	0.19992 (10)	0.0298 (5)
H62	0.2162	0.3310	0.2059	0.036*
C63	0.09012 (14)	0.3083 (2)	0.17591 (11)	0.0379 (6)
H63	0.0776	0.3980	0.1660	0.045*
C64	0.02607 (14)	0.2183 (2)	0.16628 (10)	0.0332 (5)
H64	−0.0302	0.2461	0.1505	0.040*
C65	0.04448 (13)	0.0876 (2)	0.17972 (10)	0.0286 (5)
H65	0.0008	0.0251	0.1723	0.034*
C66	0.12634 (13)	0.04734 (19)	0.20402 (9)	0.0243 (5)
H66	0.1386	−0.0427	0.2131	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0166 (9)	0.0197 (8)	0.0161 (8)	−0.0019 (7)	0.0032 (7)	−0.0008 (6)
C2	0.0157 (11)	0.0172 (9)	0.0165 (9)	0.0023 (8)	0.0027 (8)	0.0029 (8)
N3	0.0158 (9)	0.0198 (8)	0.0158 (8)	0.0005 (7)	0.0042 (7)	−0.0007 (6)
C4	0.0173 (10)	0.0153 (9)	0.0161 (9)	0.0016 (8)	0.0043 (8)	0.0035 (8)

C5	0.0177 (11)	0.0167 (9)	0.0174 (9)	−0.0010 (8)	0.0040 (8)	−0.0003 (7)
C6	0.0191 (11)	0.0137 (9)	0.0184 (9)	−0.0012 (8)	0.0019 (8)	0.0016 (7)
N21	0.0154 (9)	0.0330 (9)	0.0185 (8)	0.0004 (8)	0.0050 (7)	−0.0074 (7)
N41	0.0169 (9)	0.0256 (9)	0.0184 (8)	−0.0036 (7)	0.0064 (7)	−0.0059 (7)
C42	0.0162 (11)	0.0292 (11)	0.0200 (10)	−0.0025 (9)	0.0047 (8)	−0.0071 (8)
C43	0.0206 (11)	0.0264 (11)	0.0249 (10)	−0.0054 (9)	0.0071 (9)	−0.0073 (9)
C44	0.0229 (12)	0.0200 (10)	0.0229 (10)	−0.0003 (9)	0.0039 (9)	−0.0021 (8)
O44	0.0261 (9)	0.0387 (9)	0.0284 (8)	−0.0022 (7)	0.0069 (6)	−0.0152 (7)
O45	0.0171 (8)	0.0299 (7)	0.0231 (7)	−0.0034 (6)	0.0057 (6)	−0.0063 (6)
C46	0.0200 (12)	0.0330 (12)	0.0289 (11)	0.0026 (10)	0.0091 (9)	−0.0043 (9)
C47	0.0220 (12)	0.0389 (12)	0.0325 (12)	−0.0034 (10)	0.0088 (10)	−0.0035 (10)
C51	0.0227 (11)	0.0246 (10)	0.0185 (10)	−0.0053 (9)	0.0038 (9)	−0.0016 (8)
O51	0.0227 (8)	0.0387 (8)	0.0256 (7)	−0.0064 (7)	0.0114 (6)	−0.0071 (6)
N61	0.0194 (9)	0.0221 (8)	0.0173 (8)	−0.0024 (7)	0.0042 (7)	−0.0050 (7)
C67	0.0253 (12)	0.0315 (11)	0.0216 (10)	−0.0059 (10)	0.0075 (9)	−0.0091 (9)
C61	0.0198 (11)	0.0251 (11)	0.0155 (9)	−0.0030 (9)	0.0017 (8)	−0.0023 (8)
C62	0.0275 (13)	0.0260 (11)	0.0290 (11)	−0.0064 (10)	−0.0036 (9)	−0.0001 (9)
C63	0.0366 (14)	0.0264 (12)	0.0392 (13)	0.0024 (11)	−0.0086 (11)	0.0008 (10)
C64	0.0252 (13)	0.0342 (13)	0.0325 (12)	0.0044 (11)	−0.0048 (10)	−0.0041 (10)
C65	0.0239 (12)	0.0310 (12)	0.0280 (11)	−0.0068 (10)	0.0022 (9)	−0.0057 (9)
C66	0.0256 (12)	0.0213 (10)	0.0243 (10)	−0.0031 (9)	0.0039 (9)	−0.0044 (8)

Geometric parameters (Å, º)

N1—C6	1.339 (2)	C46—H46A	0.9900
N1—C2	1.361 (2)	C46—H46B	0.9900
C2—N21	1.340 (2)	C47—H47A	0.9800
C2—N3	1.341 (2)	C47—H47B	0.9800
N3—C4	1.346 (2)	C47—H47C	0.9800
C4—N41	1.343 (2)	C51—O51	1.239 (2)
C4—C5	1.433 (2)	C51—H51	0.9500
C5—C6	1.428 (2)	N61—C61	1.442 (2)
C5—C51	1.432 (3)	N61—C67	1.477 (2)
C6—N61	1.381 (2)	C67—H67A	0.9800
N21—H21A	0.9013	C67—H67B	0.9800
N21—H21B	0.9681	C67—H67C	0.9800
N41—C42	1.458 (2)	C61—C66	1.386 (3)
N41—H41	0.9621	C61—C62	1.390 (3)
C42—C43	1.539 (3)	C62—C63	1.389 (3)
C42—H42A	0.9900	C62—H62	0.9500
C42—H42B	0.9900	C63—C64	1.384 (3)
C43—C44	1.502 (3)	C63—H63	0.9500
C43—H43A	0.9900	C64—C65	1.381 (3)
C43—H43B	0.9900	C64—H64	0.9500
C44—O44	1.214 (2)	C65—C66	1.384 (3)
C44—O45	1.336 (2)	C65—H65	0.9500
O45—C46	1.458 (2)	C66—H66	0.9500
C46—C47	1.508 (3)		
C6—N1—C2	116.26 (15)	O45—C46—H46B	110.5

N21—C2—N3	117.27 (16)	C47—C46—H46B	110.5
N21—C2—N1	115.56 (15)	H46A—C46—H46B	108.7
N3—C2—N1	127.13 (17)	C46—C47—H47A	109.5
C2—N3—C4	116.14 (15)	C46—C47—H47B	109.5
N41—C4—N3	118.17 (16)	H47A—C47—H47B	109.5
N41—C4—C5	119.46 (16)	C46—C47—H47C	109.5
N3—C4—C5	122.37 (16)	H47A—C47—H47C	109.5
C6—C5—C51	123.02 (17)	H47B—C47—H47C	109.5
C6—C5—C4	115.02 (16)	O51—C51—C5	125.68 (18)
C51—C5—C4	121.59 (16)	O51—C51—H51	117.2
N1—C6—N61	116.47 (16)	C5—C51—H51	117.2
N1—C6—C5	122.34 (17)	C6—N61—C61	121.03 (15)
N61—C6—C5	121.18 (17)	C6—N61—C67	119.00 (16)
C2—N21—H21A	120.5	C61—N61—C67	113.12 (15)
C2—N21—H21B	118.6	N61—C67—H67A	109.5
H21A—N21—H21B	120.9	N61—C67—H67B	109.5
C4—N41—C42	124.28 (16)	H67A—C67—H67B	109.5
C4—N41—H41	118.8	N61—C67—H67C	109.5
C42—N41—H41	116.9	H67A—C67—H67C	109.5
N41—C42—C43	112.82 (16)	H67B—C67—H67C	109.5
N41—C42—H42A	109.0	C66—C61—C62	119.71 (19)
C43—C42—H42A	109.0	C66—C61—N61	120.02 (17)
N41—C42—H42B	109.0	C62—C61—N61	120.20 (17)
C43—C42—H42B	109.0	C63—C62—C61	119.50 (19)
H42A—C42—H42B	107.8	C63—C62—H62	120.2
C44—C43—C42	113.03 (16)	C61—C62—H62	120.2
C44—C43—H43A	109.0	C64—C63—C62	120.7 (2)
C42—C43—H43A	109.0	C64—C63—H63	119.7
C44—C43—H43B	109.0	C62—C63—H63	119.7
C42—C43—H43B	109.0	C65—C64—C63	119.5 (2)
H43A—C43—H43B	107.8	C65—C64—H64	120.2
O44—C44—O45	123.48 (18)	C63—C64—H64	120.2
O44—C44—C43	124.76 (18)	C64—C65—C66	120.27 (19)
O45—C44—C43	111.76 (16)	C64—C65—H65	119.9
C44—O45—C46	117.21 (14)	C66—C65—H65	119.9
O45—C46—C47	106.03 (15)	C65—C66—C61	120.27 (19)
O45—C46—H46A	110.5	C65—C66—H66	119.9
C47—C46—H46A	110.5	C61—C66—H66	119.9

C6—N1—C2—N21	176.77 (15)	O44—C44—O45—C46	0.0 (3)
C6—N1—C2—N3	−5.7 (3)	C43—C44—O45—C46	179.43 (16)
N21—C2—N3—C4	−178.63 (15)	C44—O45—C46—C47	−174.16 (16)
N1—C2—N3—C4	3.8 (3)	C6—C5—C51—O51	−174.25 (18)
C2—N3—C4—N41	−176.31 (15)	C4—C5—C51—O51	13.2 (3)
C2—N3—C4—C5	4.2 (2)	N1—C6—N61—C61	−141.21 (17)
N41—C4—C5—C6	171.17 (16)	C5—C6—N61—C61	39.4 (2)
N3—C4—C5—C6	−9.3 (2)	N1—C6—N61—C67	7.8 (2)
N41—C4—C5—C51	−15.7 (3)	C5—C6—N61—C67	−171.57 (16)
N3—C4—C5—C51	163.79 (17)	C6—N61—C61—C66	−131.94 (18)

C2—N1—C6—N61	−179.91 (15)	C67—N61—C61—C66	77.4 (2)
C2—N1—C6—C5	−0.5 (2)	C6—N61—C61—C62	51.1 (2)
C51—C5—C6—N1	−165.64 (17)	C67—N61—C61—C62	−99.6 (2)
C4—C5—C6—N1	7.4 (2)	C66—C61—C62—C63	2.3 (3)
C51—C5—C6—N61	13.7 (3)	N61—C61—C62—C63	179.22 (17)
C4—C5—C6—N61	−173.28 (16)	C61—C62—C63—C64	−0.8 (3)
N3—C4—N41—C42	3.2 (3)	C62—C63—C64—C65	−1.0 (3)
C5—C4—N41—C42	−177.28 (16)	C63—C64—C65—C66	1.4 (3)
C4—N41—C42—C43	114.35 (19)	C64—C65—C66—C61	0.1 (3)
N41—C42—C43—C44	74.4 (2)	C62—C61—C66—C65	−1.9 (3)
C42—C43—C44—O44	111.1 (2)	N61—C61—C66—C65	−178.87 (16)
C42—C43—C44—O45	−68.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21—H21*A*···N1^{i}	0.90	2.14	3.027 (2)	169
N21—H21*B*···O44^{ii}	0.97	2.14	3.054 (2)	158
N41—H41···O51	0.96	1.95	2.683 (2)	131

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

(IV) Methyl *N*-{2-amino-6-[benzyl(methyl)amino]-5-formylpyrimidin-4-yl}glycinate

Crystal data

$C_{16}H_{19}N_5O_3$
M_r = 329.36
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 15.636 (4) Å
b = 6.5674 (18) Å
c = 17.336 (5) Å
β = 113.440 (18)°
V = 1633.3 (8) Å^3
Z = 4
$F(000)$ = 696
D_x = 1.339 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3733 reflections
θ = 2.8–27.5°
μ = 0.10 mm^{-1}
T = 120 K
Block, colourless
0.29 × 0.27 × 0.15 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
Radiation source: Bruker Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.973, T_{max} = 0.986
21188 measured reflections
3013 independent reflections
2209 reflections with $I > 2\sigma(I)$
R_{int} = 0.072
θ_{max} = 25.5°, θ_{min} = 2.8°
h = −18→18
k = −7→7
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.165
S = 1.09
3013 reflections
219 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

$w = 1/[\sigma^2(F_o^2) + (0.0897P)^2 + 1.0498P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.76191 (13)	0.7943 (3)	0.53404 (12)	0.0198 (5)
C2	0.82036 (15)	0.6345 (4)	0.56416 (14)	0.0182 (5)
N3	0.85110 (13)	0.5052 (3)	0.52088 (11)	0.0186 (5)
C4	0.83019 (15)	0.5560 (4)	0.44062 (13)	0.0170 (5)
C5	0.77674 (15)	0.7337 (4)	0.40234 (14)	0.0191 (5)
C6	0.73816 (16)	0.8387 (4)	0.45326 (14)	0.0184 (5)
N21	0.84767 (14)	0.5969 (3)	0.64650 (12)	0.0227 (5)
H21A	0.8254	0.6764	0.6840	0.027*
H21B	0.8675	0.4707	0.6640	0.027*
N41	0.86339 (14)	0.4372 (3)	0.39645 (12)	0.0216 (5)
H41	0.8525	0.4819	0.3409	0.026*
C42	0.92283 (16)	0.2643 (4)	0.43330 (14)	0.0206 (5)
H42A	0.8894	0.1646	0.4540	0.025*
H42B	0.9793	0.3093	0.4816	0.025*
C43	0.94983 (16)	0.1673 (4)	0.36808 (14)	0.0193 (5)
O43	0.91642 (11)	0.2078 (3)	0.29407 (10)	0.0231 (4)
O44	1.01581 (12)	0.0275 (3)	0.40347 (10)	0.0258 (4)
C45	1.04556 (18)	−0.0855 (4)	0.34677 (16)	0.0268 (6)
H45A	1.0646	0.0098	0.3131	0.040*
H45B	0.9939	−0.1696	0.3095	0.040*
H45C	1.0983	−0.1731	0.3794	0.040*
C51	0.77698 (15)	0.8161 (4)	0.32669 (14)	0.0200 (5)
H51	0.7535	0.9504	0.3121	0.024*
O51	0.80517 (12)	0.7278 (3)	0.27814 (10)	0.0262 (4)
N61	0.67418 (14)	0.9937 (3)	0.42083 (12)	0.0220 (5)
C67	0.59484 (17)	0.9692 (4)	0.33873 (15)	0.0246 (6)
H67A	0.6164	0.8947	0.3001	0.029*
H67B	0.5735	1.1055	0.3143	0.029*
C61	0.51365 (17)	0.8562 (4)	0.34467 (15)	0.0221 (5)
C62	0.52537 (18)	0.6637 (4)	0.38099 (16)	0.0285 (6)
H62	0.5858	0.6047	0.4040	0.034*
C63	0.45071 (19)	0.5564 (5)	0.38425 (17)	0.0320 (6)
H63	0.4601	0.4251	0.4093	0.038*
C64	0.36207 (18)	0.6408 (5)	0.35094 (17)	0.0327 (7)
H64	0.3106	0.5678	0.3531	0.039*
C65	0.34922 (18)	0.8310 (5)	0.31483 (18)	0.0360 (7)
H65	0.2886	0.8891	0.2919	0.043*
C66	0.42394 (17)	0.9384 (5)	0.31163 (16)	0.0292 (6)
H66	0.4140	1.0698	0.2866	0.035*
C68	0.65143 (18)	1.1154 (4)	0.48056 (16)	0.0283 (6)
H68A	0.7090	1.1536	0.5280	0.042*

H68B	0.6119	1.0356	0.5012	0.042*
H68C	0.6181	1.2386	0.4526	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0178 (10)	0.0224 (11)	0.0180 (10)	0.0019 (8)	0.0059 (8)	0.0006 (8)
C2	0.0139 (11)	0.0219 (13)	0.0185 (11)	−0.0020 (10)	0.0062 (9)	−0.0016 (10)
N3	0.0181 (10)	0.0218 (11)	0.0152 (10)	0.0001 (8)	0.0061 (8)	−0.0007 (8)
C4	0.0122 (11)	0.0216 (13)	0.0153 (11)	−0.0016 (9)	0.0037 (9)	−0.0005 (9)
C5	0.0132 (11)	0.0233 (13)	0.0187 (11)	−0.0012 (10)	0.0043 (9)	0.0004 (10)
C6	0.0156 (11)	0.0196 (13)	0.0186 (11)	−0.0025 (9)	0.0052 (9)	−0.0009 (9)
N21	0.0268 (11)	0.0249 (12)	0.0166 (10)	0.0053 (9)	0.0090 (8)	0.0016 (8)
N41	0.0231 (11)	0.0256 (12)	0.0156 (9)	0.0056 (9)	0.0071 (8)	0.0023 (8)
C42	0.0201 (12)	0.0231 (13)	0.0168 (11)	0.0016 (10)	0.0052 (9)	−0.0011 (10)
C43	0.0191 (12)	0.0175 (13)	0.0206 (12)	−0.0016 (10)	0.0072 (10)	−0.0007 (9)
O43	0.0254 (9)	0.0269 (10)	0.0166 (8)	0.0016 (7)	0.0079 (7)	−0.0002 (7)
O44	0.0280 (10)	0.0291 (10)	0.0190 (8)	0.0097 (8)	0.0079 (7)	0.0003 (7)
C45	0.0275 (13)	0.0291 (15)	0.0238 (12)	0.0077 (11)	0.0102 (11)	−0.0031 (11)
C51	0.0125 (11)	0.0251 (14)	0.0194 (11)	0.0003 (10)	0.0031 (9)	0.0021 (10)
O51	0.0284 (10)	0.0332 (11)	0.0195 (8)	0.0013 (8)	0.0121 (7)	0.0041 (8)
N61	0.0182 (10)	0.0239 (12)	0.0202 (10)	0.0030 (9)	0.0037 (8)	−0.0002 (8)
C67	0.0209 (13)	0.0276 (15)	0.0210 (12)	0.0059 (11)	0.0039 (10)	0.0057 (10)
C61	0.0199 (12)	0.0270 (14)	0.0164 (11)	0.0012 (10)	0.0040 (9)	−0.0020 (10)
C62	0.0206 (13)	0.0313 (16)	0.0293 (13)	0.0005 (11)	0.0054 (11)	0.0013 (12)
C63	0.0286 (14)	0.0346 (16)	0.0292 (13)	−0.0062 (12)	0.0078 (11)	−0.0005 (12)
C64	0.0235 (14)	0.0464 (19)	0.0289 (14)	−0.0103 (13)	0.0111 (11)	−0.0123 (13)
C65	0.0167 (13)	0.054 (2)	0.0329 (15)	0.0023 (12)	0.0051 (11)	−0.0084 (14)
C66	0.0227 (13)	0.0344 (16)	0.0267 (13)	0.0076 (11)	0.0057 (11)	0.0017 (11)
C68	0.0239 (13)	0.0282 (15)	0.0286 (13)	0.0077 (11)	0.0061 (11)	−0.0033 (11)

Geometric parameters (Å, º)

N1—C6	1.331 (3)	C45—H45C	0.9800
N1—C2	1.353 (3)	C51—O51	1.239 (3)
C2—N21	1.340 (3)	C51—H51	0.9500
C2—N3	1.342 (3)	N61—C68	1.459 (3)
N3—C4	1.339 (3)	N61—C67	1.479 (3)
C4—N41	1.334 (3)	C67—C61	1.509 (4)
C4—C5	1.436 (3)	C67—H67A	0.9900
C5—C51	1.420 (3)	C67—H67B	0.9900
C5—C6	1.429 (3)	C61—C62	1.392 (4)
C6—N61	1.381 (3)	C61—C66	1.396 (4)
N21—H21A	0.9984	C62—C63	1.383 (4)
N21—H21B	0.8951	C62—H62	0.9500
N41—C42	1.445 (3)	C63—C64	1.387 (4)
N41—H41	0.9547	C63—H63	0.9500
C42—C43	1.497 (3)	C64—C65	1.376 (5)
C42—H42A	0.9900	C64—H64	0.9500
C42—H42B	0.9900	C65—C66	1.385 (4)

C43—O43	1.207 (3)	C65—H65	0.9500
C43—O44	1.334 (3)	C66—H66	0.9500
O44—C45	1.448 (3)	C68—H68A	0.9800
C45—H45A	0.9800	C68—H68B	0.9800
C45—H45B	0.9800	C68—H68C	0.9800

C6—N1—C2	116.0 (2)	O51—C51—C5	125.5 (2)
N21—C2—N3	116.5 (2)	O51—C51—H51	117.2
N21—C2—N1	115.7 (2)	C5—C51—H51	117.2
N3—C2—N1	127.8 (2)	C6—N61—C68	117.2 (2)
C4—N3—C2	115.4 (2)	C6—N61—C67	120.4 (2)
N41—C4—N3	117.4 (2)	C68—N61—C67	113.3 (2)
N41—C4—C5	119.9 (2)	N61—C67—C61	113.2 (2)
N3—C4—C5	122.7 (2)	N61—C67—H67A	108.9
C51—C5—C6	122.9 (2)	C61—C67—H67A	108.9
C51—C5—C4	121.5 (2)	N61—C67—H67B	108.9
C6—C5—C4	114.7 (2)	C61—C67—H67B	108.9
N1—C6—N61	116.3 (2)	H67A—C67—H67B	107.7
N1—C6—C5	122.3 (2)	C62—C61—C66	117.8 (2)
N61—C6—C5	121.3 (2)	C62—C61—C67	121.0 (2)
C2—N21—H21A	123.5	C66—C61—C67	121.1 (2)
C2—N21—H21B	116.9	C63—C62—C61	121.3 (3)
H21A—N21—H21B	115.2	C63—C62—H62	119.3
C4—N41—C42	122.29 (19)	C61—C62—H62	119.3
C4—N41—H41	116.4	C62—C63—C64	119.9 (3)
C42—N41—H41	120.8	C62—C63—H63	120.0
N41—C42—C43	108.99 (18)	C64—C63—H63	120.0
N41—C42—H42A	109.9	C65—C64—C63	119.5 (3)
C43—C42—H42A	109.9	C65—C64—H64	120.2
N41—C42—H42B	109.9	C63—C64—H64	120.2
C43—C42—H42B	109.9	C64—C65—C66	120.5 (3)
H42A—C42—H42B	108.3	C64—C65—H65	119.7
O43—C43—O44	124.7 (2)	C66—C65—H65	119.7
O43—C43—C42	125.2 (2)	C65—C66—C61	120.8 (3)
O44—C43—C42	110.13 (19)	C65—C66—H66	119.6
C43—O44—C45	116.03 (18)	C61—C66—H66	119.6
O44—C45—H45A	109.5	N61—C68—H68A	109.5
O44—C45—H45B	109.5	N61—C68—H68B	109.5
H45A—C45—H45B	109.5	H68A—C68—H68B	109.5
O44—C45—H45C	109.5	N61—C68—H68C	109.5
H45A—C45—H45C	109.5	H68A—C68—H68C	109.5
H45B—C45—H45C	109.5	H68B—C68—H68C	109.5

C6—N1—C2—N21	176.8 (2)	O43—C43—O44—C45	−2.2 (4)
C6—N1—C2—N3	−6.0 (4)	C42—C43—O44—C45	177.2 (2)
N21—C2—N3—C4	−174.1 (2)	C6—C5—C51—O51	−176.2 (2)
N1—C2—N3—C4	8.8 (4)	C4—C5—C51—O51	15.3 (4)
C2—N3—C4—N41	176.7 (2)	N1—C6—N61—C68	10.2 (3)
C2—N3—C4—C5	−1.4 (3)	C5—C6—N61—C68	−169.3 (2)

N41—C4—C5—C51	−15.8 (3)	N1—C6—N61—C67	−134.4 (2)
N3—C4—C5—C51	162.2 (2)	C5—C6—N61—C67	46.0 (3)
N41—C4—C5—C6	174.8 (2)	C6—N61—C67—C61	83.0 (3)
N3—C4—C5—C6	−7.2 (3)	C68—N61—C67—C61	−63.0 (3)
C2—N1—C6—N61	176.2 (2)	N61—C67—C61—C62	−55.3 (3)
C2—N1—C6—C5	−4.2 (3)	N61—C67—C61—C66	126.7 (2)
C51—C5—C6—N1	−159.1 (2)	C66—C61—C62—C63	0.1 (4)
C4—C5—C6—N1	10.1 (3)	C67—C61—C62—C63	−177.9 (2)
C51—C5—C6—N61	20.4 (4)	C61—C62—C63—C64	−0.1 (4)
C4—C5—C6—N61	−170.3 (2)	C62—C63—C64—C65	0.0 (4)
N3—C4—N41—C42	−2.4 (3)	C63—C64—C65—C66	−0.1 (4)
C5—C4—N41—C42	175.7 (2)	C64—C65—C66—C61	0.2 (4)
C4—N41—C42—C43	−178.5 (2)	C62—C61—C66—C65	−0.2 (4)
N41—C42—C43—O43	−10.1 (3)	C67—C61—C66—C65	177.9 (2)
N41—C42—C43—O44	170.47 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21—H21*A*···O51^{i}	1.00	1.89	2.860 (3)	163
N21—H21*B*···O43^{ii}	0.89	2.38	3.085 (3)	136
N41—H41···O51	0.96	1.92	2.682 (3)	135

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2; (ii) *x*, −*y*+1/2, *z*+1/2.

(V) Ethyl 3-amino-*N*-{2-amino-6-[benzyl(methyl)amino]-5-formylpyrimidin- 4-yl}propionate

Crystal data

$C_{18}H_{23}N_5O_3$
M_r = 357.41
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 24.8226 (5) Å
b = 7.1379 (14) Å
c = 20.601 (2) Å
β = 106.213 (8)°
V = 3505.0 (8) Å^3
Z = 8
F(000) = 1520
D_x = 1.355 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 4039 reflections
θ = 3.0–27.5°
μ = 0.10 mm^{-1}
T = 120 K
Block, colourless
0.26 × 0.21 × 0.14 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
Radiation source: Bruker Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.976, T_{max} = 0.987
22384 measured reflections
3269 independent reflections
2276 reflections with $I > 2\sigma(I)$
R_{int} = 0.073
θ_{max} = 25.5°, θ_{min} = 3.0°
h = −30→30
k = −8→8
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.104$
$S = 1.06$
3269 reflections
237 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
$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 2.9368P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.69278 (6)	0.7477 (2)	0.66478 (8)	0.0163 (4)
C2	0.70537 (8)	0.6127 (3)	0.71219 (10)	0.0154 (4)
N3	0.67234 (6)	0.4705 (2)	0.72058 (8)	0.0166 (4)
C4	0.62542 (8)	0.4445 (3)	0.66962 (10)	0.0159 (4)
C5	0.61274 (8)	0.5559 (3)	0.60889 (10)	0.0169 (4)
C6	0.64576 (8)	0.7221 (3)	0.61344 (9)	0.0157 (4)
N21	0.75599 (6)	0.6237 (2)	0.75782 (8)	0.0188 (4)
H21A	0.7798	0.7296	0.7585	0.023*
H21B	0.7679	0.5267	0.7903	0.023*
N41	0.59084 (7)	0.3046 (2)	0.67526 (8)	0.0200 (4)
H41	0.5572	0.2751	0.6363	0.024*
C42	0.59488 (8)	0.1981 (3)	0.73683 (10)	0.0202 (5)
H42A	0.5670	0.2466	0.7588	0.024*
H42B	0.6326	0.2161	0.7685	0.024*
C43	0.58472 (8)	−0.0093 (3)	0.72265 (10)	0.0202 (5)
H43A	0.6123	−0.0571	0.7001	0.024*
H43B	0.5907	−0.0769	0.7660	0.024*
C44	0.52655 (8)	−0.0493 (3)	0.67878 (10)	0.0191 (5)
O44	0.49263 (6)	0.0690 (2)	0.65309 (9)	0.0387 (4)
O45	0.51667 (6)	−0.23223 (19)	0.67155 (7)	0.0267 (4)
C46	0.46236 (9)	−0.2905 (3)	0.62757 (11)	0.0288 (5)
H46A	0.4650	−0.3114	0.5810	0.035*
H46B	0.4339	−0.1924	0.6262	0.035*
C47	0.44631 (9)	−0.4687 (3)	0.65593 (12)	0.0328 (6)
H47A	0.4763	−0.5613	0.6606	0.049*
H47B	0.4115	−0.5174	0.6254	0.049*
H47C	0.4406	−0.4438	0.7003	0.049*
C51	0.57391 (8)	0.4903 (3)	0.54831 (10)	0.0210 (5)
H51	0.5723	0.5570	0.5079	0.025*
O51	0.54207 (6)	0.35380 (19)	0.54367 (7)	0.0249 (4)
N61	0.63127 (6)	0.8638 (2)	0.56785 (8)	0.0173 (4)
C67	0.67035 (8)	1.0176 (3)	0.56761 (10)	0.0199 (5)
H67A	0.7071	0.9885	0.5999	0.024*
H67B	0.6560	1.1337	0.5831	0.024*
C61	0.67824 (8)	1.0504 (3)	0.49824 (10)	0.0197 (5)

C62	0.68991 (9)	0.9001 (3)	0.46137 (11)	0.0258 (5)
H62	0.6899	0.7762	0.4782	0.031*
C63	0.70159 (9)	0.9299 (4)	0.40034 (11)	0.0333 (6)
H63	0.7097	0.8266	0.3756	0.040*
C64	0.70148 (9)	1.1090 (4)	0.37540 (11)	0.0343 (6)
H64	0.7095	1.1290	0.3335	0.041*
C65	0.68969 (9)	1.2590 (3)	0.41123 (11)	0.0318 (6)
H65	0.6894	1.3824	0.3939	0.038*
C66	0.67813 (8)	1.2301 (3)	0.47289 (11)	0.0243 (5)
H66	0.6701	1.3338	0.4976	0.029*
C68	0.57405 (8)	0.8987 (3)	0.52501 (10)	0.0215 (5)
H68A	0.5714	0.8621	0.4784	0.032*
H68B	0.5653	1.0323	0.5264	0.032*
H68C	0.5474	0.8251	0.5417	0.032*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0162 (8)	0.0174 (9)	0.0144 (9)	0.0005 (7)	0.0028 (7)	0.0001 (8)
C2	0.0154 (10)	0.0149 (10)	0.0159 (11)	0.0020 (8)	0.0042 (9)	−0.0031 (9)
N3	0.0153 (8)	0.0175 (9)	0.0157 (9)	0.0010 (7)	0.0024 (7)	0.0005 (7)
C4	0.0151 (10)	0.0141 (10)	0.0190 (11)	0.0031 (8)	0.0054 (9)	−0.0038 (9)
C5	0.0163 (10)	0.0163 (10)	0.0174 (10)	0.0016 (8)	0.0037 (8)	0.0007 (9)
C6	0.0164 (10)	0.0174 (11)	0.0147 (10)	0.0022 (8)	0.0064 (8)	−0.0017 (9)
N21	0.0172 (9)	0.0170 (9)	0.0187 (9)	−0.0023 (7)	−0.0008 (7)	0.0034 (8)
N41	0.0197 (9)	0.0184 (9)	0.0192 (9)	−0.0027 (7)	0.0010 (7)	0.0029 (8)
C42	0.0221 (11)	0.0207 (11)	0.0179 (11)	−0.0028 (9)	0.0057 (9)	0.0007 (9)
C43	0.0194 (10)	0.0214 (11)	0.0201 (11)	0.0007 (9)	0.0063 (9)	0.0022 (9)
C44	0.0239 (11)	0.0160 (11)	0.0192 (11)	−0.0015 (9)	0.0092 (9)	0.0002 (9)
O44	0.0252 (8)	0.0215 (8)	0.0587 (12)	0.0003 (7)	−0.0059 (8)	0.0012 (8)
O45	0.0260 (8)	0.0172 (8)	0.0320 (9)	−0.0039 (6)	0.0002 (7)	0.0003 (7)
C46	0.0284 (12)	0.0281 (13)	0.0265 (13)	−0.0098 (10)	0.0018 (10)	−0.0015 (11)
C47	0.0292 (12)	0.0231 (13)	0.0433 (15)	−0.0040 (10)	0.0057 (11)	0.0028 (11)
C51	0.0218 (11)	0.0167 (11)	0.0217 (11)	0.0049 (9)	0.0017 (9)	0.0019 (10)
O51	0.0244 (8)	0.0170 (8)	0.0266 (9)	−0.0045 (6)	−0.0040 (7)	−0.0007 (7)
N61	0.0167 (8)	0.0172 (9)	0.0164 (9)	−0.0020 (7)	0.0021 (7)	0.0032 (8)
C67	0.0217 (10)	0.0201 (11)	0.0167 (11)	−0.0035 (9)	0.0032 (9)	−0.0006 (9)
C61	0.0138 (10)	0.0246 (12)	0.0184 (11)	−0.0025 (9)	0.0006 (8)	0.0036 (10)
C62	0.0259 (11)	0.0276 (13)	0.0239 (12)	0.0003 (10)	0.0069 (10)	0.0003 (10)
C63	0.0277 (12)	0.0487 (15)	0.0252 (13)	−0.0016 (11)	0.0102 (10)	−0.0055 (12)
C64	0.0243 (12)	0.0607 (18)	0.0190 (12)	−0.0039 (12)	0.0076 (10)	0.0082 (12)
C65	0.0211 (11)	0.0412 (15)	0.0309 (13)	−0.0026 (11)	0.0034 (10)	0.0187 (12)
C66	0.0180 (10)	0.0260 (12)	0.0274 (12)	−0.0004 (9)	0.0040 (9)	0.0054 (10)
C68	0.0193 (11)	0.0190 (11)	0.0234 (12)	0.0011 (9)	0.0012 (9)	0.0023 (9)

Geometric parameters (Å, º)

N1—C2	1.346 (2)	C46—H46B	0.9900
N1—C6	1.351 (2)	C47—H47A	0.9800
C2—N21	1.345 (2)	C47—H47B	0.9800

C2—N3	1.346 (2)	C47—H47C	0.9800
N3—C4	1.346 (2)	C51—O51	1.241 (2)
C4—N41	1.343 (2)	C51—H51	0.9500
C4—C5	1.441 (3)	N61—C67	1.466 (2)
C5—C51	1.426 (3)	N61—C68	1.469 (2)
C5—C6	1.430 (3)	C67—C61	1.514 (3)
C6—N61	1.359 (2)	C67—H67A	0.9900
N21—H21A	0.9568	C67—H67B	0.9900
N21—H21B	0.9506	C61—C66	1.384 (3)
N41—C42	1.458 (2)	C61—C62	1.391 (3)
N41—H41	1.0067	C62—C63	1.383 (3)
C42—C43	1.516 (3)	C62—H62	0.9500
C42—H42A	0.9900	C63—C64	1.377 (3)
C42—H42B	0.9900	C63—H63	0.9500
C43—C44	1.501 (3)	C64—C65	1.378 (3)
C43—H43A	0.9900	C64—H64	0.9500
C43—H43B	0.9900	C65—C66	1.394 (3)
C44—O44	1.205 (2)	C65—H65	0.9500
C44—O45	1.330 (2)	C66—H66	0.9500
O45—C46	1.459 (2)	C68—H68A	0.9800
C46—C47	1.499 (3)	C68—H68B	0.9800
C46—H46A	0.9900	C68—H68C	0.9800

C2—N1—C6	116.49 (16)	C46—C47—H47A	109.5
N21—C2—N1	116.59 (17)	C46—C47—H47B	109.5
N21—C2—N3	115.99 (17)	H47A—C47—H47B	109.5
N1—C2—N3	127.38 (17)	C46—C47—H47C	109.5
C4—N3—C2	115.43 (16)	H47A—C47—H47C	109.5
N41—C4—N3	118.03 (17)	H47B—C47—H47C	109.5
N41—C4—C5	119.71 (17)	O51—C51—C5	125.83 (19)
N3—C4—C5	122.21 (17)	O51—C51—H51	117.1
C51—C5—C6	124.40 (18)	C5—C51—H51	117.1
C51—C5—C4	120.58 (18)	C6—N61—C67	120.81 (16)
C6—C5—C4	114.74 (17)	C6—N61—C68	124.49 (16)
N1—C6—N61	116.39 (17)	C67—N61—C68	113.63 (15)
N1—C6—C5	121.19 (17)	N61—C67—C61	112.29 (16)
N61—C6—C5	122.41 (17)	N61—C67—H67A	109.1
C2—N21—H21A	120.6	C61—C67—H67A	109.1
C2—N21—H21B	119.7	N61—C67—H67B	109.1
H21A—N21—H21B	119.8	C61—C67—H67B	109.1
C4—N41—C42	124.93 (17)	H67A—C67—H67B	107.9
C4—N41—H41	119.7	C66—C61—C62	119.17 (19)
C42—N41—H41	115.2	C66—C61—C67	120.82 (19)
N41—C42—C43	111.95 (16)	C62—C61—C67	119.84 (18)
N41—C42—H42A	109.2	C63—C62—C61	120.4 (2)
C43—C42—H42A	109.2	C63—C62—H62	119.8
N41—C42—H42B	109.2	C61—C62—H62	119.8
C43—C42—H42B	109.2	C64—C63—C62	120.2 (2)
H42A—C42—H42B	107.9	C64—C63—H63	119.9

C44—C43—C42	112.44 (17)	C62—C63—H63	119.9
C44—C43—H43A	109.1	C63—C64—C65	120.0 (2)
C42—C43—H43A	109.1	C63—C64—H64	120.0
C44—C43—H43B	109.1	C65—C64—H64	120.0
C42—C43—H43B	109.1	C64—C65—C66	120.1 (2)
H43A—C43—H43B	107.8	C64—C65—H65	119.9
O44—C44—O45	123.66 (19)	C66—C65—H65	119.9
O44—C44—C43	124.59 (19)	C61—C66—C65	120.1 (2)
O45—C44—C43	111.75 (17)	C61—C66—H66	119.9
C44—O45—C46	117.33 (16)	C65—C66—H66	119.9
O45—C46—C47	107.45 (17)	N61—C68—H68A	109.5
O45—C46—H46A	110.2	N61—C68—H68B	109.5
C47—C46—H46A	110.2	H68A—C68—H68B	109.5
O45—C46—H46B	110.2	N61—C68—H68C	109.5
C47—C46—H46B	110.2	H68A—C68—H68C	109.5
H46A—C46—H46B	108.5	H68B—C68—H68C	109.5

C6—N1—C2—N21	170.68 (16)	O44—C44—O45—C46	2.7 (3)
C6—N1—C2—N3	−11.6 (3)	C43—C44—O45—C46	−177.40 (16)
N21—C2—N3—C4	−170.86 (16)	C44—O45—C46—C47	−147.25 (18)
N1—C2—N3—C4	11.4 (3)	C6—C5—C51—O51	−174.98 (18)
C2—N3—C4—N41	−179.97 (16)	C4—C5—C51—O51	11.5 (3)
C2—N3—C4—C5	2.7 (3)	N1—C6—N61—C67	11.4 (2)
N41—C4—C5—C51	−17.6 (3)	C5—C6—N61—C67	−170.05 (17)
N3—C4—C5—C51	159.69 (18)	N1—C6—N61—C68	−156.05 (17)
N41—C4—C5—C6	168.26 (16)	C5—C6—N61—C68	22.5 (3)
N3—C4—C5—C6	−14.5 (3)	C6—N61—C67—C61	128.48 (18)
C2—N1—C6—N61	176.14 (16)	C68—N61—C67—C61	−62.8 (2)
C2—N1—C6—C5	−2.5 (3)	N61—C67—C61—C66	135.72 (19)
C51—C5—C6—N1	−159.69 (18)	N61—C67—C61—C62	−49.1 (2)
C4—C5—C6—N1	14.2 (3)	C66—C61—C62—C63	0.4 (3)
C51—C5—C6—N61	21.8 (3)	C67—C61—C62—C63	−174.87 (19)
C4—C5—C6—N61	−164.31 (17)	C61—C62—C63—C64	−0.3 (3)
N3—C4—N41—C42	11.0 (3)	C62—C63—C64—C65	0.0 (3)
C5—C4—N41—C42	−171.62 (17)	C63—C64—C65—C66	0.3 (3)
C4—N41—C42—C43	−138.69 (18)	C62—C61—C66—C65	−0.1 (3)
N41—C42—C43—C44	−63.1 (2)	C67—C61—C66—C65	175.10 (18)
C42—C43—C44—O44	5.3 (3)	C64—C65—C66—C61	−0.2 (3)
C42—C43—C44—O45	−174.63 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21—H21*A*···N3^{i}	0.96	2.07	3.008 (2)	168
N21—H21*B*···N1^{ii}	0.95	2.30	3.199 (2)	158
N41—H41···O44	1.01	2.27	2.891 (2)	119
N41—H41···O51	1.01	1.92	2.666 (2)	128
C46—H46*A*···O51^{iii}	0.99	2.54	3.528 (3)	172

Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+3/2; (ii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iii) −*x*+1, −*y*, −*z*+1.

(VI) ethyl 3-amino-*N*-[2-amino-5-formyl-6-(piperidin-4-yl)pyrimidin-4-yl]propionate

Crystal data

$C_{15}H_{23}N_5O_3$
$M_r = 321.38$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.040$ (4) Å
$b = 10.391$ (3) Å
$c = 10.458$ (8) Å
$\alpha = 109.16$ (3)°
$\beta = 98.19$ (5)°
$\gamma = 103.10$ (3)°
$V = 781.2$ (8) Å^3
$Z = 2$
$F(000) = 344$
$D_x = 1.366$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3583 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.10$ mm^{-1}
$T = 120$ K
Block, colourless
0.41 × 0.25 × 0.22 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
Radiation source: Bruker–Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.885$, $T_{max} = 0.936$
17622 measured reflections
3227 independent reflections
2384 reflections with $I > 2\sigma(I)$
$R_{int} = 0.059$
$\theta_{max} = 26.5°$, $\theta_{min} = 2.9°$
$h = -10 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.134$
$S = 1.05$
3227 reflections
209 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
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 0.5988P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.2067 (2)	0.99862 (17)	0.39947 (17)	0.0181 (4)
C2	0.1344 (3)	0.8952 (2)	0.2717 (2)	0.0178 (4)
N3	0.0811 (2)	0.75376 (17)	0.23960 (17)	0.0177 (4)
C4	0.0706 (3)	0.7141 (2)	0.3481 (2)	0.0171 (4)
C5	0.1156 (3)	0.8157 (2)	0.48841 (19)	0.0172 (4)
C6	0.2032 (3)	0.9578 (2)	0.5067 (2)	0.0178 (4)
N21	0.1241 (2)	0.93797 (18)	0.16430 (17)	0.0221 (4)
H21A	0.1448	1.0307	0.1857	0.027*
H21B	0.0549	0.8723	0.0841	0.027*
N41	0.0112 (2)	0.57444 (17)	0.32114 (17)	0.0186 (4)
H41	0.0086	0.5442	0.3960	0.022*
C42	−0.0436 (3)	0.4661 (2)	0.18126 (19)	0.0182 (4)

H42A	−0.1151	0.4985	0.1199	0.022*
H42B	−0.1192	0.3776	0.1834	0.022*
C43	0.1089 (3)	0.4326 (2)	0.1192 (2)	0.0212 (4)
H43A	0.0686	0.3906	0.0164	0.025*
H43B	0.2036	0.5225	0.1446	0.025*
C44	0.1820 (3)	0.3315 (2)	0.1681 (2)	0.0196 (4)
O44	0.10635 (19)	0.20552 (14)	0.12956 (14)	0.0223 (3)
O45	0.34111 (19)	0.39256 (14)	0.25435 (14)	0.0222 (3)
C46	0.4207 (3)	0.2999 (2)	0.3051 (2)	0.0257 (5)
H46A	0.4186	0.2144	0.2260	0.031*
H46B	0.3549	0.2685	0.3679	0.031*
C47	0.6066 (3)	0.3843 (2)	0.3820 (3)	0.0312 (5)
H47A	0.6071	0.4713	0.4567	0.047*
H47B	0.6722	0.4097	0.3174	0.047*
H47C	0.6618	0.3270	0.4223	0.047*
C51	0.0490 (3)	0.7813 (2)	0.5944 (2)	0.0192 (4)
H51	0.0596	0.8579	0.6784	0.023*
O51	−0.02206 (19)	0.65980 (14)	0.58706 (14)	0.0216 (3)
N61	0.2857 (2)	1.05882 (17)	0.63761 (17)	0.0199 (4)
C62	0.3611 (3)	1.2063 (2)	0.6514 (2)	0.0218 (5)
H62A	0.2834	1.2294	0.5853	0.026*
H62B	0.4769	1.2169	0.6275	0.026*
C63	0.3831 (3)	1.3095 (2)	0.7991 (2)	0.0248 (5)
H63A	0.2658	1.3073	0.8187	0.030*
H63B	0.4419	1.4074	0.8071	0.030*
C64	0.4915 (3)	1.2721 (2)	0.9069 (2)	0.0257 (5)
H64A	0.6140	1.2870	0.8961	0.031*
H64B	0.4935	1.3350	1.0019	0.031*
C65	0.4114 (3)	1.1178 (2)	0.8867 (2)	0.0264 (5)
H65A	0.4866	1.0916	0.9517	0.032*
H65B	0.2941	1.1056	0.9080	0.032*
C66	0.3942 (3)	1.0207 (2)	0.7381 (2)	0.0216 (5)
H66A	0.5125	1.0283	0.7191	0.026*
H66B	0.3396	0.9207	0.7262	0.026*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0212 (9)	0.0155 (8)	0.0162 (8)	0.0040 (7)	0.0016 (7)	0.0064 (7)
C2	0.0191 (10)	0.0160 (9)	0.0169 (10)	0.0048 (8)	0.0016 (8)	0.0059 (8)
N3	0.0197 (9)	0.0163 (8)	0.0169 (8)	0.0038 (7)	0.0021 (7)	0.0077 (7)
C4	0.0170 (10)	0.0168 (9)	0.0184 (10)	0.0061 (8)	0.0021 (8)	0.0078 (8)
C5	0.0202 (10)	0.0155 (9)	0.0146 (9)	0.0042 (8)	0.0001 (8)	0.0061 (8)
C6	0.0186 (10)	0.0161 (9)	0.0186 (10)	0.0062 (8)	0.0015 (8)	0.0066 (8)
N21	0.0298 (10)	0.0152 (8)	0.0179 (8)	0.0024 (7)	−0.0006 (7)	0.0072 (7)
N41	0.0266 (9)	0.0144 (8)	0.0144 (8)	0.0053 (7)	0.0021 (7)	0.0063 (7)
C42	0.0222 (10)	0.0155 (9)	0.0150 (10)	0.0040 (8)	0.0009 (8)	0.0056 (8)
C43	0.0290 (11)	0.0174 (10)	0.0165 (10)	0.0048 (8)	0.0034 (8)	0.0075 (8)
C44	0.0248 (11)	0.0186 (10)	0.0140 (9)	0.0051 (8)	0.0054 (8)	0.0047 (8)
O44	0.0281 (8)	0.0156 (7)	0.0195 (7)	0.0038 (6)	0.0004 (6)	0.0057 (6)

O45	0.0235 (8)	0.0193 (7)	0.0223 (7)	0.0050 (6)	0.0019 (6)	0.0082 (6)
C46	0.0277 (12)	0.0228 (11)	0.0271 (11)	0.0087 (9)	0.0009 (9)	0.0112 (9)
C47	0.0244 (12)	0.0315 (12)	0.0334 (13)	0.0098 (10)	0.0018 (10)	0.0076 (10)
C51	0.0210 (10)	0.0188 (10)	0.0166 (10)	0.0066 (8)	0.0017 (8)	0.0059 (8)
O51	0.0265 (8)	0.0189 (7)	0.0201 (7)	0.0041 (6)	0.0049 (6)	0.0099 (6)
N61	0.0244 (9)	0.0140 (8)	0.0172 (8)	0.0025 (7)	−0.0005 (7)	0.0050 (7)
C62	0.0272 (11)	0.0149 (10)	0.0187 (10)	0.0018 (8)	0.0003 (9)	0.0055 (8)
C63	0.0299 (12)	0.0166 (10)	0.0209 (11)	0.0027 (9)	0.0007 (9)	0.0032 (8)
C64	0.0306 (12)	0.0205 (10)	0.0176 (10)	0.0026 (9)	−0.0014 (9)	0.0030 (8)
C65	0.0327 (12)	0.0242 (11)	0.0183 (10)	0.0042 (9)	0.0006 (9)	0.0078 (9)
C66	0.0239 (11)	0.0185 (10)	0.0201 (10)	0.0055 (8)	−0.0007 (8)	0.0074 (8)

Geometric parameters (Å, º)

N1—C6	1.324 (3)	C46—H46A	0.9900
N1—C2	1.353 (3)	C46—H46B	0.9900
C2—N21	1.336 (3)	C47—H47A	0.9800
C2—N3	1.344 (3)	C47—H47B	0.9800
N3—C4	1.335 (3)	C47—H47C	0.9800
C4—N41	1.339 (3)	C51—O51	1.234 (2)
C4—C5	1.434 (3)	C51—H51	0.9500
C5—C51	1.409 (3)	N61—C62	1.465 (3)
C5—C6	1.421 (3)	N61—C66	1.481 (3)
C6—N61	1.378 (3)	C62—C63	1.522 (3)
N21—H21A	0.8843	C62—H62A	0.9900
N21—H21B	0.8932	C62—H62B	0.9900
N41—C42	1.453 (3)	C63—C64	1.530 (3)
N41—H41	0.9356	C63—H63A	0.9900
C42—C43	1.522 (3)	C63—H63B	0.9900
C42—H42A	0.9900	C64—C65	1.517 (3)
C42—H42B	0.9900	C64—H64A	0.9900
C43—C44	1.502 (3)	C64—H64B	0.9900
C43—H43A	0.9900	C65—C66	1.516 (3)
C43—H43B	0.9900	C65—H65A	0.9900
C44—O44	1.212 (2)	C65—H65B	0.9900
C44—O45	1.335 (3)	C66—H66A	0.9900
O45—C46	1.461 (2)	C66—H66B	0.9900
C46—C47	1.500 (3)		

C6—N1—C2	116.23 (17)	C46—C47—H47A	109.5
N21—C2—N3	116.10 (18)	C46—C47—H47B	109.5
N21—C2—N1	116.28 (18)	H47A—C47—H47B	109.5
N3—C2—N1	127.51 (18)	C46—C47—H47C	109.5
C4—N3—C2	115.03 (17)	H47A—C47—H47C	109.5
N3—C4—N41	117.39 (18)	H47B—C47—H47C	109.5
N3—C4—C5	122.16 (18)	O51—C51—C5	125.40 (19)
N41—C4—C5	120.43 (18)	O51—C51—H51	117.3
C51—C5—C6	122.24 (18)	C5—C51—H51	117.3
C51—C5—C4	121.52 (18)	C6—N61—C62	118.51 (17)
C6—C5—C4	115.25 (18)	C6—N61—C66	119.36 (16)

N1—C6—N61	117.61 (18)	C62—N61—C66	111.47 (16)
N1—C6—C5	121.51 (18)	N61—C62—C63	111.02 (17)
N61—C6—C5	120.87 (18)	N61—C62—H62A	109.4
C2—N21—H21A	115.9	C63—C62—H62A	109.4
C2—N21—H21B	114.8	N61—C62—H62B	109.4
H21A—N21—H21B	123.6	C63—C62—H62B	109.4
C4—N41—C42	123.41 (17)	H62A—C62—H62B	108.0
C4—N41—H41	118.7	C62—C63—C64	111.73 (18)
C42—N41—H41	117.9	C62—C63—H63A	109.3
N41—C42—C43	113.62 (17)	C64—C63—H63A	109.3
N41—C42—H42A	108.8	C62—C63—H63B	109.3
C43—C42—H42A	108.8	C64—C63—H63B	109.3
N41—C42—H42B	108.8	H63A—C63—H63B	107.9
C43—C42—H42B	108.8	C65—C64—C63	109.64 (18)
H42A—C42—H42B	107.7	C65—C64—H64A	109.7
C44—C43—C42	112.97 (17)	C63—C64—H64A	109.7
C44—C43—H43A	109.0	C65—C64—H64B	109.7
C42—C43—H43A	109.0	C63—C64—H64B	109.7
C44—C43—H43B	109.0	H64A—C64—H64B	108.2
C42—C43—H43B	109.0	C66—C65—C64	110.45 (18)
H43A—C43—H43B	107.8	C66—C65—H65A	109.6
O44—C44—O45	122.99 (19)	C64—C65—H65A	109.6
O44—C44—C43	123.36 (19)	C66—C65—H65B	109.6
O45—C44—C43	113.62 (17)	C64—C65—H65B	109.6
C44—O45—C46	116.48 (16)	H65A—C65—H65B	108.1
O45—C46—C47	107.34 (18)	N61—C66—C65	111.06 (17)
O45—C46—H46A	110.2	N61—C66—H66A	109.4
C47—C46—H46A	110.2	C65—C66—H66A	109.4
O45—C46—H46B	110.2	N61—C66—H66B	109.4
C47—C46—H46B	110.2	C65—C66—H66B	109.4
H46A—C46—H46B	108.5	H66A—C66—H66B	108.0

C6—N1—C2—N21	174.38 (18)	C42—C43—C44—O44	72.8 (3)
C6—N1—C2—N3	−9.8 (3)	C42—C43—C44—O45	−109.4 (2)
N21—C2—N3—C4	−171.57 (18)	O44—C44—O45—C46	−1.7 (3)
N1—C2—N3—C4	12.6 (3)	C43—C44—O45—C46	−179.55 (17)
C2—N3—C4—N41	177.37 (17)	C44—O45—C46—C47	171.90 (18)
C2—N3—C4—C5	−0.8 (3)	C6—C5—C51—O51	−177.03 (19)
N3—C4—C5—C51	157.28 (19)	C4—C5—C51—O51	14.9 (3)
N41—C4—C5—C51	−20.9 (3)	N1—C6—N61—C62	4.2 (3)
N3—C4—C5—C6	−11.6 (3)	C5—C6—N61—C62	−174.97 (18)
N41—C4—C5—C6	170.27 (18)	N1—C6—N61—C66	−137.42 (19)
C2—N1—C6—N61	175.91 (17)	C5—C6—N61—C66	43.4 (3)
C2—N1—C6—C5	−5.0 (3)	C6—N61—C62—C63	158.54 (18)
C51—C5—C6—N1	−154.2 (2)	C66—N61—C62—C63	−57.0 (2)
C4—C5—C6—N1	14.6 (3)	N61—C62—C63—C64	55.0 (2)
C51—C5—C6—N61	24.9 (3)	C62—C63—C64—C65	−53.9 (3)
C4—C5—C6—N61	−166.31 (18)	C63—C64—C65—C66	55.0 (3)
N3—C4—N41—C42	−0.9 (3)	C6—N61—C66—C65	−156.94 (19)

C5—C4—N41—C42	177.40 (18)	C62—N61—C66—C65	59.0 (2)
C4—N41—C42—C43	78.2 (2)	C64—C65—C66—N61	−58.0 (2)
N41—C42—C43—C44	81.2 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N21—H21*A*···O44^{i}	0.88	2.15	2.951 (3)	150
N21—H21*B*···O44^{ii}	0.89	2.20	3.036 (3)	156
N41—H41···O51	0.94	2.05	2.700 (3)	125
N41—H41···O51^{iii}	0.94	2.21	2.909 (3)	131
C43—H43*A*···N3^{ii}	0.99	2.55	3.524 (4)	169

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

Selected geometric parameters (Å, °) for compounds (I)–(VI)

(i)	Bond lengths					
Parameter	(I)	(II)	(III)	(IV)	(V)	(VI)
N1—C2	1.353 (2)	1.350 (3)	1.361 (2)	1.353 (3)	1.346 (2)	1.353 (3)
C2—N3	1.340 (2)	1.352 (3)	1.341 (2)	1.342 (3)	1.346 (2)	1.344 (2)
N3—C4	1.335 (2)	1.336 (3)	1.346 (2)	1.339 (3)	1.346 (2)	1.335 (3)
C4—C5	1.430 (2)	1.436 (3)	1.433 (2)	1.436 (3)	1.441 (3)	1.434 (3)
C5—C6	1.418 (2)	1.438 (3)	1.428 (2)	1.429 (3)	1.430 (3)	1.421 (3)
C6—N1	1.335 (2)	1.336 (3)	1.339 (2)	1.331 (3)	1.351 (2)	1.324 (3)
C2—N21	1.342 (2)	1.337 (3)	1.340 (2)	1.340 (3)	1.345 (2)	1.336 (3)
C4—N41	1.336 (2)	1.352 (3)	1.343 (2)	1.334 (3)	1.343 (2)	1.339 (3)
C5—C51	1.426 (3)	1.426 (3)	1.432 (3)	1.420 (3)	1.426 (3)	1.409 (3)
C51—O51	1.232 (2)	1.247 (3)	1.239 (2)	1.239 (3)	1.241 (2)	1.234 (2)
C6—N61	1.380 (2)	1.371 (3)	1.381 (2)	1.381 (3)	1.359 (2)	1.378 (3)
(ii)	Torsion angles					
N3—C4—N41—C42	-4.8 (2)	7.0 (3)	3.2 (3)	-2.4 (3)	11.0 (3)	-0.9 (3)
C4—N41—C42—C43	-196.15 (17)	-88.6 (3)	114.35 (19)	-178.5 (2)	-138.69 (18)	78.2 (2)
N41—C42—C43—C44			74.4 (2)		-63.1 (2)	81.2 (2)
N41—C42—C43—N44		1.3 (3)				
N41—C42—C43—O44	-172.71 (17)			170.47 (19)		
C42—C43—C44—O45			-68.3 (2)		-174.63 (16)	-109.4 (2)
C43—C44—O45—C46			179.43 (16)		-177.40 (16)	-179.55 (17)
C44—O45—C46—C47			-174.16 (16)		-147.25 (18)	171.90 (18)
C42—C43—O44—C45	178.29 (17)			177.2 (2)		
C43—O44—C45—C46	170.04 (19)					

C4—C5—C51—O51	13.1 (3)	8.3 (4)	13.2 (3)	15.3 (4)	11.5 (3)	14.9 (3)
C5—C6—N61—C61	42.6 (3)	35.4 (3)	39.4 (2)			
C5—C6—N61—C62						-174.97 (18)
C5—C6—N61—C66						43.4 (3)
C5—C6—N61—C67	-161.27 (18)	-175.8 (2)	-171.57 (16)	46.0 (3)	-170.05 (17)	
C5—C6—C61—C68				-169.3 (2)	22.5 (3)	

(iii) Substituent displacement from mean pyrimidine plane

Compound	N21	N41	C51	O51	N61
(I)	0.077 (2)	-0.015 (2)	0.319 (2)	0.334 (2)	-0.071 (2)
(II)	0.132 (2)	-0.035 (2)	0.321 (2)	0.391 (2)	-0.101 (2)
(III)	0.106 (2)	-0.162 (2)	0.353 (2)	0.331 (2)	-0.084 (2)
(IV)	0.161 (2)	-0.037 (2)	0.444 (3)	0.487 (2)	-0.190 (2)
(V)	0.300 (2)	-0.172 (2)	0.493 (2)	0.548 (2)	-0.256 (2)
(VI)	0.245 (2)	-0.104 (2)	0.564 (2)	0.670 (2)	-0.251 (2)

(iv) Ring-puckering parameters

Compound	*Q*	*θ*	*φ*
(IV)	0.100 (3)	97.0 (17)	76.9 (14)
(V)	0.156 (3)	98.5 (7)	59.8 (7)
(VI)	0.149 (2)	96.9 (8)	71.8 (8)
Idealized boat		90.0	60*n*

Hydrogen bonds and short intramolecular contacts (Å, °) for compounds (I)–(VI)

Compound	*D*—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
(I)	N21—H21*A*···N1^{i}	0.92	2.22	3.125 (2)	167
	N41—H41···O51	0.94	1.90	2.675 (2)	138
(II)	N21—H21*A*···O43^{ii}	0.94	2.02	2.933 (2)	166
	N41—H41···O51	0.90	1.98	2.689 (2)	135
	N44—H44*A*···O51^{iii}	0.95	2.14	2.949 (2)	143
	N44—H44*B*···O43^{iv}	0.98	2.05	3.006 (3)	164
	C62—H62···O43^{v}	0.95	2.45	3.280 (3)	146
(III)	N21—H21*A*···N1^{iii}	0.90	2.14	3.027 (2)	169
	N21—H21*B*···O44^{v}	0.97	2.14	3.054 (2)	158

	N41—H41···O51	0.96	1.95	2.683 (2)	131
(IV)	N21—H21*A*···O51^{vi}	1.00	1.89	2.860 (3)	163
	N21—H21*B*···O43^{vii}	0.89	2.38	3.085 (3)	136
	N41—H41···O51	0.96	1.92	2.682 (3)	135
(V)	N21—H21*A*···N3^{viii}	0.96	2.07	3.008 (2)	168
	N21—H21*B*···N1^{ix}	0.95	2.30	3.199 (2)	158
	N41—H41···O44	1.01	2.27	2.891 (2)	119
	N41—H41···O51	1.01	1.92	2.666 (2)	128
	C46—H46*A*···O51^{x}	0.99	2.54	3.528 (3)	172
(VI)	N21—H21*A*···O44^{ii}	0.88	2.15	2.951 (3)	150
	N21—H21*B*···O44^{xi}	0.89	2.20	3.036 (3)	156
	N41—H41···O51	0.94	2.05	2.700 (3)	125
	N41—H41···O51^{i}	0.94	2.21	2.909 (3)	131
	C43—H43*A*···N3^{xi}	0.99	2.55	3.524 (4)	169

Symmetry codes: (i) -x, -y + 1, -z + 1; (ii) x, y + 1, z; (iii) -x + 1, y, -z + 1/2; (iv) -x + 3/2, -y + 1/2, -z + 1; (v) -x + 1, -y + 1, -z + 1; (vi) x, -y + 3/2, z + 1/2; (vii) x, -y + 1/2, z + 1/2; (viii) -x + 3/2, y + 1/2, -z + 3/2; (ix) -x + 3/2, y - 1/2, -z + 3/2; (x) -x + 1, -y, -z + 1; (xi) -x, -y + 1, -z.