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Design of two series of 1:1 cocrystals involving 4-amino-5-chloro-2,6-dimethylpyrimidine and carboxylic acids

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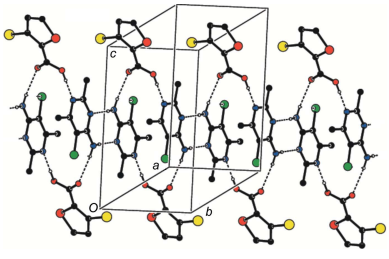
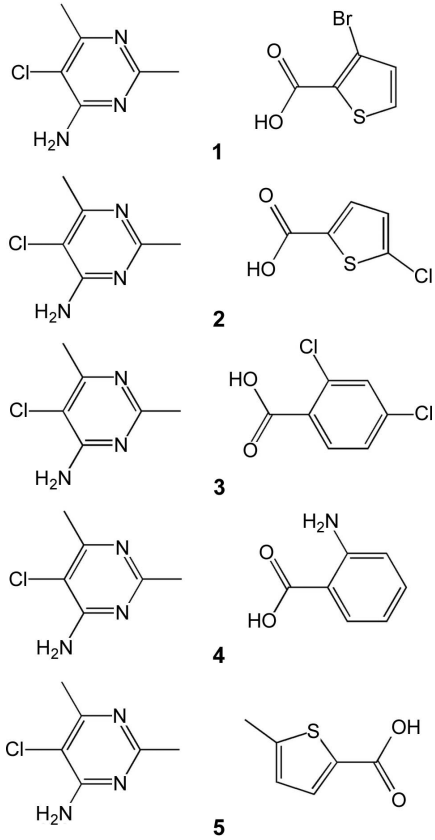
Two series of a total of ten cocrystals involving 4-amino-5-chloro-2,6-dimethylpyrimidine with various carboxylic acids have been prepared and characterized by single-crystal X-ray diffraction. The pyrimidine unit used for the cocrystals offers two ring N atoms (positions N1 and N3) as proton-accepting sites. Depending upon the site of protonation, two types of cations are possible [Rajam *et al.* (2017). *Acta Cryst.* C**73**, 862–868]. In a parallel arrangement, two series of cocrystals are possible depending upon the hydrogen bonding of the carboxyl group with position N1 or N3. In one series of cocrystals, *i.e.* 4-amino-5-chloro-2,6-dimethylpyrimidine–3-bromothiophene-2-carboxylic acid (1/1), **1**, 4-amino-5-chloro-2,6-dimethylpyrimidine–5-chlorothiophene-2-carboxylic acid (1/1), **2**, 4-amino-5-chloro-2,6-dimethylpyrimidine–2,4-dichlorobenzoic acid (1/1), **3**, and 4-amino-5-chloro-2,6-dimethylpyrimidine–2-aminobenzoic acid (1/1), **4**, the carboxyl hydroxy group (–OH) is hydrogen bonded to position N1 (O—H···N1) of the corresponding pyrimidine unit (single point supramolecular synthon). The inversion-related stacked pyrimidines are doubly bridged by the carboxyl groups *via* N—H···O and O—H···N hydrogen bonds to form a large cage-like tetrameric unit with an $R_4^2(20)$ graph-set ring motif. These tetrameric units are further connected *via* base pairing through a pair of N—H···N hydrogen bonds, generating $R_2^2(8)$ motifs (supramolecular homosynthon). In the other series of cocrystals, *i.e.* 4-amino-5-chloro-2,6-dimethylpyrimidine–5-methylthiophene-2-carboxylic acid (1/1), **5**, 4-amino-5-chloro-2,6-dimethylpyrimidine–benzoic acid (1/1), **6**, 4-amino-5-chloro-2,6-dimethylpyrimidine–2-methylbenzoic acid (1/1), **7**, 4-amino-5-chloro-2,6-dimethylpyrimidine–3-methylbenzoic acid (1/1), **8**, 4-amino-5-chloro-2,6-dimethylpyrimidine–4-methylbenzoic acid (1/1), **9**, and 4-amino-5-chloro-2,6-dimethylpyrimidine–4-aminobenzoic acid (1/1), **10**, the carboxyl group interacts with position N3 and the adjacent 4-amino group of the corresponding pyrimidine ring *via* O—H···N and N—H···O hydrogen bonds to generate the robust $R_2^2(8)$ supramolecular heterosynthon. These heterosynthons are further connected by N—H···N hydrogen-bond interactions in a linear fashion to form a chain-like arrangement. In cocrystal **1**, a Br···Br halogen bond is present, in cocrystals **2** and **3**, Cl···Cl halogen bonds are present, and in cocrystals **5**, **6** and **7**, Cl···O halogen bonds are present. In all of the ten cocrystals, π–π stacking interactions are observed.



1. Introduction

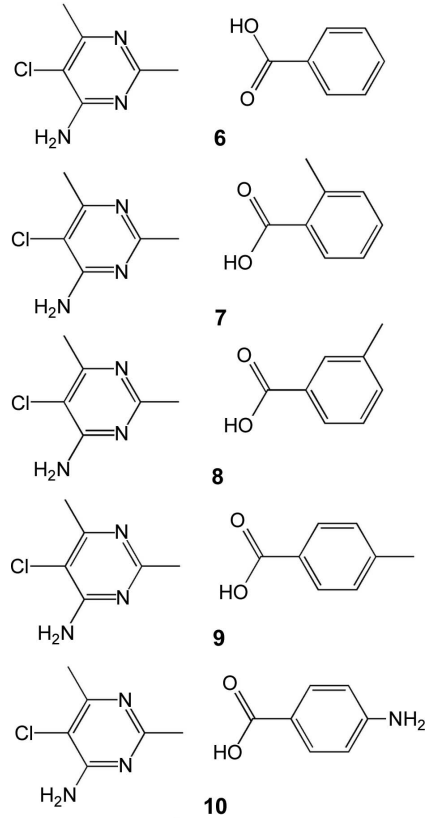
In crystal engineering, noncovalent interactions such as hydrogen bonds, halogen bonds, anion–π, cation–π and π–π interactions, together with other weak forces, play a central role in the self-assembly and molecular recognition processes (García-Raso *et al.*, 2009; Aakeröy *et al.*, 2009; Nandi *et al.*, 2014). In particular, halogen bonding is of current interest and exhibits a wide range of applications, such as in catalysis,

medicinal chemistry and structural chemistry (Cavallo *et al.*, 2016; Metrangolo & Resnati, 2012). Recently, much consideration has been given to the synthesis of cocrystals related to their wide-ranging applications in the pharmaceutical industry (Zhu *et al.*, 2015; Griffini *et al.*, 2014; Baldrighi *et al.*, 2013). Pyrimidines and aminopyrimidine derivatives are biologically important compounds as they are distributed widely in nature as components of nucleic acids and drugs (Selvam *et al.*, 2012; Sharma *et al.*, 2014). In crystal engineering, carboxylic acid is one of the most commonly used functional groups and hence the formation of robust heterosynthons from the carboxylic acid–pyrimidine moiety has attracted much attention. The pyrimidine–carboxylic acid interaction is also involved in protein–nucleic acid binding and drug–protein recognition processes. Hydrogen-bonding patterns, including base pairing formed by the aminopyrimidines, are important in the structure and functions of nucleic acids (Stanley *et al.*, 2002; Baskar Raj *et al.*, 2003). The hydrogen-bonding patterns present in several aminopyrimidine–carboxylates and cocrystals have been reported by us (Ebenezer *et al.*, 2011; Tamilselvi & Muthiah, 2011; Ebenezer & Muthiah, 2012; Jegan Jennifer & Muthiah, 2014; Karthikeyan *et al.*, 2015; Rajam *et al.*, 2015, 2017; Swinton Darious *et al.*, 2017).



Scheme 1

In the present study, we have synthesized and structurally characterized two series of a total of ten cocrystals, namely 4-amino-5-chloro-2,6-dimethylpyrimidine–3-bromothiophene-2-carboxylic acid (1/1), **1**, 4-amino-5-chloro-2,6-dimethylpyrimidine–5-chlorothiophene-2-carboxylic acid (1/1), **2**, 4-amino-5-chloro-2,6-dimethylpyrimidine–2,4-dichlorobenzoic acid (1/1), **3**, 4-amino-5-chloro-2,6-dimethylpyrimidine–2-aminobenzoic acid (1/1), **4**, 4-amino-5-chloro-2,6-dimethylpyrimidine–5-methylthiophene-2-carboxylic acid (1/1), **5**, 4-amino-5-chloro-2,6-dimethylpyrimidine–benzoic acid (1/1), **6**, 4-amino-5-chloro-2,6-dimethylpyrimidine–2-methylbenzoic acid (1/1), **7**, 4-amino-5-chloro-2,6-dimethylpyrimidine–3-methylbenzoic acid (1/1), **8**, 4-amino-5-chloro-2,6-dimethylpyrimidine–4-methylbenzoic acid (1/1), **9**, and 4-amino-5-chloro-2,6-dimethylpyrimidine–4-aminobenzoic acid (1/1), **10**. Depending on the nature and position of the substituent present in the carboxylic acids, the carboxyl hydroxy group (–OH) is hydogen bonded to atom N1 (O—H···N1) of the corresponding pyrimidine ring, *i.e.* crystal structures **1**–**4**. Atom N1 is flanked by the methyl groups present in the pyrimidine moiety, so a robust heterosynthon motif formation is not possible. For crystal structures **5**–**10**, the carboxyl group interacts with atom N3 and the adjacent 4-amino group of the corresponding pyrimidine ring *via* O—H···N and N—H···O hydrogen bonds to generate the robust $R_2^2(8)$ supramolecular heterosynthon.



Scheme 2

2. Experimental

2.1. Synthesis and crystallization

2.1.1. Cocrystal 1. 4-Amino-5-chloro-2,6-dimethylpyrimidine (39 mg) and 3-bromothiophene-2-carboxylic acid (51 mg) were dissolved in a hot acetonitrile solution (1:1 molar ratio) and warmed over a water bath for half an hour. The resulting clear solution was allowed to evaporate. After a few days,

Table 1
Experimental details.

For all determinations, H atoms were treated by a mixture of independent and constrained refinement.

	1	**2**	**3**	**4**
Crystal data				
Chemical formula	$C_5H_3BrO_2S·C_6H_8ClN_3$	$C_6H_8ClN_3·C_5H_3ClO_2S$	$C_6H_8ClN_3·C_7H_4Cl_2O_2$	$C_6H_8ClN_3·C_7H_7NO_2$
M_r	364.65	320.19	348.61	294.74
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/n$
Temperature (K)	100	100	120	120
a, b, c (Å)	7.5237 (4), 7.5739 (4), 12.5089 (7)	7.2182 (3), 7.6364 (3), 12.7516 (6)	7.3015 (4), 7.5060 (6), 14.9665 (8)	8.0965 (2), 7.2427 (3), 24.0738 (9)
α, β, γ (°)	79.629 (2), 79.596 (2), 75.895 (2)	90.707 (2), 102.629 (2), 105.338 (2)	92.539 (5), 98.522 (5), 113.657 (7)	90, 90.831 (3), 90
V (Å^3)	673.00 (6)	659.61 (5)	738.12 (9)	1411.55 (9)
Z	2	2	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	3.41	0.65	5.70	2.47
Crystal size (mm)	0.31 × 0.27 × 0.21	0.37 × 0.19 × 0.11	0.51 × 0.35 × 0.08	0.46 × 0.22 × 0.06
Data collection				
Diffractometer	Bruker D8 Quest CMOS	Bruker D8 Quest CMOS	Agilent SuperNova Dual Source diffractometer with an Atlas detector	Agilent SuperNova Dual Source diffractometer with an Atlas detector
Absorption correction	Multi-scan (*APEX2*; Bruker, 2014)	Multi-scan (*APEX2*; Bruker, 2014)	Multi-scan (*CrysAlis PRO*; Agilent, 2014)	Analytical [*CrysAlis PRO* (Oxford Diffraction, 2011), based on expressions derived by Clark & Reid (1995)]
T_{min}, T_{max}	0.539, 0.747	0.477, 0.746	0.538, 1.000	0.547, 0.877
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13063, 5103, 4471	8796, 3636, 2947	5965, 3050, 2546	6899, 2927, 2481
R_{int}	0.032	0.051	0.038	0.028
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.770	0.695	0.632	0.631
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.070, 1.04	0.051, 0.138, 1.15	0.047, 0.135, 1.05	0.039, 0.110, 1.05
No. of reflections	5103	3636	3050	2927
No. of parameters	187	187	204	203
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.67, −0.52	0.76, −0.56	0.39, −0.51	0.23, −0.47

	5	**6**	**7**	**8**
Crystal data				
Chemical formula	$C_6H_8ClN_3·C_6H_6O_2S$	$C_6H_8ClN_3·C_7H_6O_2$	$C_6H_8ClN_3·C_8H_8O_2$	$C_6H_8ClN_3·C_8H_8O_2$
M_r	299.77	279.72	293.75	293.75
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $Pbcn$
Temperature (K)	100	120	120	120
a, b, c (Å)	8.273 (3), 12.746 (4), 13.320 (4)	10.1421 (5), 10.4218 (5), 13.2681 (6)	7.3992 (2), 13.9842 (4), 26.9897 (8)	8.4524 (1), 13.5387 (2), 24.9813 (3)
α, β, γ (°)	90, 102.390 (5), 90	90, 107.804 (5), 90	90, 90, 90	90, 90, 90
V (Å^3)	1371.8 (8)	1335.26 (12)	2792.68 (14)	2858.72 (6)
Z	4	4	8	8
Radiation type	Mo $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	0.43	2.56	2.47	2.42
Crystal size (mm)	0.55 × 0.50 × 0.30	0.52 × 0.38 × 0.24	0.49 × 0.11 × 0.08	0.42 × 0.24 × 0.19
Data collection				
Diffractometer	Bruker APEXII CCD	Agilent SuperNova Dual Source diffractometer with an Atlas detector	Agilent SuperNova Dual Source diffractometer with an Atlas detector	Agilent SuperNova Dual Source diffractometer with an Atlas detector
Absorption correction	Multi-scan (*APEX2*; Bruker, 2014)	Multi-scan (*CrysAlis PRO*; Agilent, 2014)	Multi-scan (*CrysAlis PRO*; Agilent, 2014)	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.608, 0.746	0.763, 1.000	0.740, 1.000	0.680, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8807, 4109, 3735	6087, 2760, 2560	8897, 4966, 4617	26401, 3006, 2904
R_{int}	0.028	0.029	0.030	0.033
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.734	0.631	0.631	0.631
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.092, 1.05	0.041, 0.118, 1.04	0.034, 0.091, 1.04	0.037, 0.103, 1.04
No. of reflections	4109	2760	4966	3006

Table 1 (continued)

	5	6	7	8
No. of parameters	189	187	376	196
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.55, −0.29	0.33, −0.44	0.24, −0.24	0.30, −0.31
Absolute structure	–	–	Flack x determined using 1451 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)	–
Absolute structure parameter	–	–	−0.001 (10)	–

	9	10
Crystal data		
Chemical formula	$C_6H_8ClN_3{\cdot}C_8H_8O_2$	$C_6H_8ClN_3{\cdot}C_7H_7NO_2$
M_r	293.75	294.74
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$
Temperature (K)	120	120
a, b, c (Å)	8.0223 (5), 13.6901 (10), 13.3346 (10)	7.8899 (2), 13.2361 (3), 13.3212 (3)
α, β, γ (°)	90, 101.557 (7), 90	90, 101.254 (2), 90
V (Å^3)	1434.80 (18)	1364.40 (6)
Z	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	2.41	2.56
Crystal size (mm)	0.51 × 0.17 × 0.08	0.41 × 0.35 × 0.24
Data collection		
Diffractometer	Agilent SuperNova Dual Source diffractometer with an Atlas detector	Agilent SuperNova Dual Source diffractometer with an Atlas detector
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.582, 1.000	0.828, 1.000
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	6765, 2966, 2422	6214, 2823, 2749
R_{int}	0.040	0.017
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.631	0.631
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.140, 1.04	0.036, 0.097, 1.04
No. of reflections	2966	2823
No. of parameters	197	203
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.41	0.27, −0.38

Computer programs: *APEX2* (Bruker, 2014), *CrysAlis PRO* (Agilent, 2014; Oxford Diffraction, 2011), *SAINT* (Bruker, 2013, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *SHELXL2014* (Sheldrick, 2015*b*), *shelXle* (Hübschle *et al.*, 2011), *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

colourless block-shaped crystals of **1** separated out from the mother liquor.

2.1.2. Cocrystal 2. 4-Amino-5-chloro-2,6-dimethylpyrimidine (39 mg) and 5-chlorothiophene-2-carboxylic acid (41 mg) were dissolved in a hot dimethylformamide (DMF) solution (1:1 molar ratio) and warmed over a water bath for half an hour. The clear solution was allowed to evaporate. After a few days, colourless block-shaped crystals of **2** separated out from the mother liquid.

2.1.3. Cocrystal 3. 4-Amino-5-chloro-2,6-dimethylpyrimidine (39 mg) and 2,4-dichlorobenzoic acid (47 mg) were dissolved in hot ethanol (1:1 molar ratio) and warmed over a water bath for half an hour. The clear solution was allowed to evaporate. After a few days, colourless crystals of **3** separated out from the mother liquid.

2.1.4. Cocrystal 4. 4-Amino-5-chloro-2,6-dimethylpyrimidine (39 mg) and 2-aminobenzoic acid (34 mg) were dissolved in hot ethanol (1:1 molar ratio) and warmed over a water bath for half an hour. The clear solution was allowed to evaporate. After a few days, pale yellow–orange crystals of **4** separated out from the mother liquid.

2.1.5. Cocrystal 5. 4-Amino-5-chloro-2,6-dimethylpyrimidine (39 mg) and 5-methylthiophene-2-carboxylic acid (35 mg) were dissolved in hot acetonitrile (1:1 molar ratio) and warmed over a water bath for half an hour. The clear solution was allowed to evaporate. After a few days, colourless plate-like crystals of **5** separated out from the mother liquid.

2.1.6. Cocrystal 6. 4-Amino-5-chloro-2,6-dimethylpyrimidine (39 mg) and benzoic acid (31 mg) were dissolved in hot methanol (1:1 molar ratio) and warmed over a water bath for half an hour. The clear solution was allowed to evaporate. After a few days, colourless crystals of **6** separated out from the mother liquid.

2.1.7. Cocrystal 7. 4-Amino-5-chloro-2,6-dimethylpyrimidine (39 mg) and 2-methylbenzoic acid (34 mg) were dissolved in hot ethanol (1:1 molar ratio) and warmed over a water bath for half an hour. The clear solution was allowed to evaporate. After a few days, colourless crystals of **7** separated out from the mother liquid.

2.1.8. Cocrystal 8. 4-Amino-5-chloro-2,6-dimethylpyrimidine (39 mg) and 3-methylbenzoic acid (34 mg) were dissolved in hot ethanol (1:1 molar ratio) and warmed over a water bath

for half an hour. The clear solution was allowed to evaporate. After a few days, colourless crystals of **8** separated out from the mother liquid.

2.1.9. Cocrystal 9. 4-Amino-5-chloro-2,6-dimethylpyrimidine (39 mg) and 4-methylbenzoic acid (34 mg) were dissolved in hot ethanol (1:1 molar ratio) and warmed over a water bath for half an hour. The clear solution was allowed to evaporate. After a few days, colourless crystals of **9** separated out from the mother liquid.

2.1.10. Cocrystal 10. 4-Amino-5-chloro-2,6-dimethylpyrimidine (39 mg) and 4-aminobenzoic acid (34 mg) were dissolved in hot ethanolic solution (1:1 molar ratio) and warmed over a water bath for half an hour. The clear solution was allowed to evaporate. After a few days, colourless crystals of **10** separated out from the mother liquid.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. For cocrystals **1**, **2** and **5**, the N—H and O—H hydrogens were located in difference Fourier maps and refined isotropically. All other H atoms were placed in calculated positions and refined using a riding-model approximation, with C—H = 0.95 (CH) or 0.98 Å (CH_3). Isotropic displacement parameters for these atoms were set at $1.2U_{eq}$ (for CH) or $1.5U_{eq}$ (for CH_3) of the parent atom. Idealized methyl H atoms were refined as rotating groups. There are larger than expected residual density peaks close to the Cl and S atoms, but these are not chemically sensible and are assumed to be related to the quality of the crystal. For crystals **3**, **4** and **6**–**10**, the N—H and O—H hydrogens were located in difference Fourier maps and refined isotropically. All other H atoms were placed in calculated positions and refined using a riding-model approximation, with C—H = 0.95 (for H) or 0.98 Å (for CH_3). Isotropic displacement parameters for these atoms were set at $1.2U_{eq}$ (for CH) or $1.5U_{eq}$ (for CH_3) of the parent atom. Idealized methyl H atoms were refined as rotating groups.

3. Results and discussion

The carboxylic acids and 4-amino-5-chloro-2,6-dimethylpyrimidine used in the present study are shown in Schemes 1 and 2. In the crystal structures of **1**–**10** (except **7**), the asymmetric unit contains a molecule of 4-amino-5-chloro-2,6-dimethylpyrimidine and a molecule of the carboxylic acid, whereas in the crystal structure of **7**, the asymmetric unit contains two molecules of the pyrimidine base and two molecules of the carboxylic acid. Views of the asymmetric units in each of the ten compounds are shown in Figs. 1–10. In all of the ten cocrystals, the carboxyl H atom was located in a difference Fourier map. The bond lengths and angles of the carboxyl group are similar to those reported for a typical carboxyl group rather than a carboxylate group. In the first series of cocrystals, *i.e.* **1**–**4**, the carboxyl hydroxy group (–OH) is hydrogen bonded to atom N1 (O—H···N1) of the corresponding pyrimidine (single point supramolecular synthon).

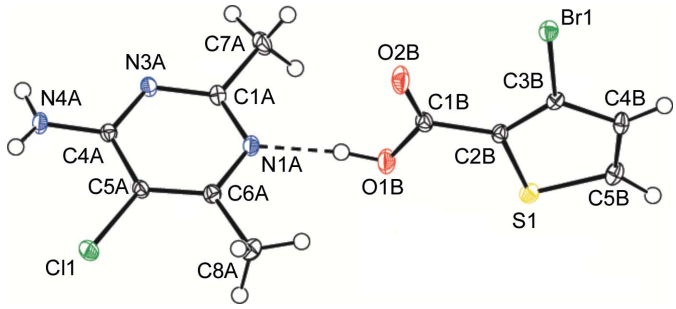


Figure 1
The asymmetric unit of cocrystal **1**, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Dashed lines represent hydrogen bonds.

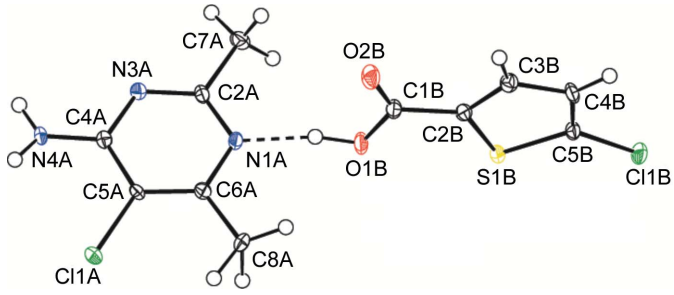


Figure 2
The asymmetric unit of cocrystal **2**, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Dashed lines represent hydrogen bonds.

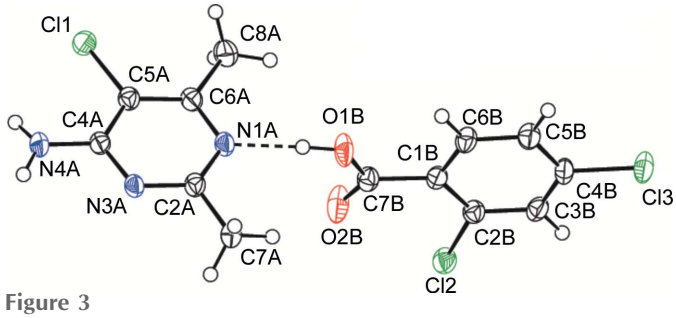


Figure 3
The asymmetric unit of cocrystal **3**, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Dashed lines represent hydrogen bonds.

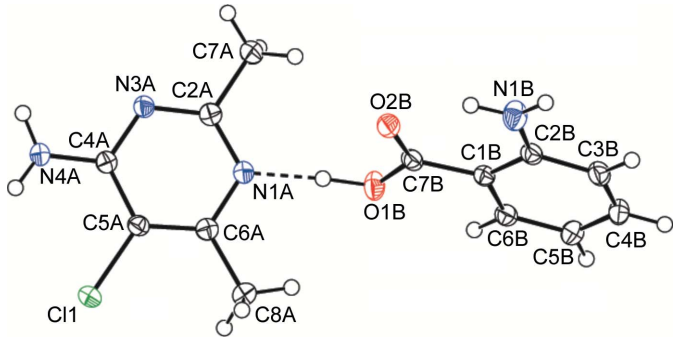


Figure 4
The asymmetric unit of cocrystal **4**, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Dashed lines represent hydrogen bonds.

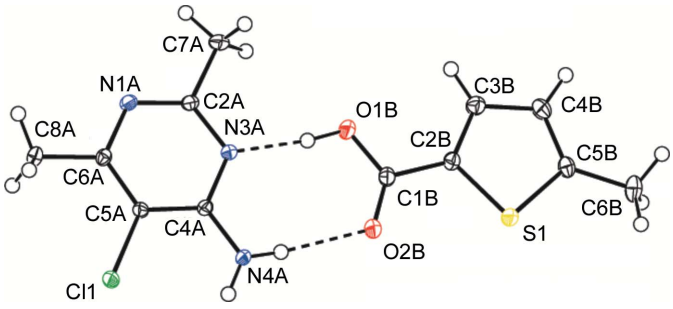


Figure 5
The asymmetric unit of cocrystal **5**, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Dashed lines represent hydrogen bonds.

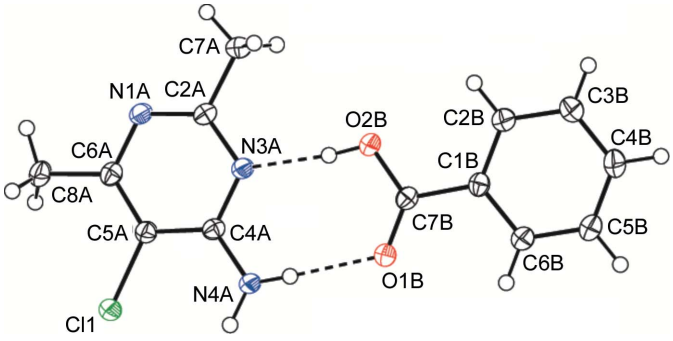


Figure 6
The asymmetric unit of cocrystal **6**, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Dashed lines represent hydrogen bonds.

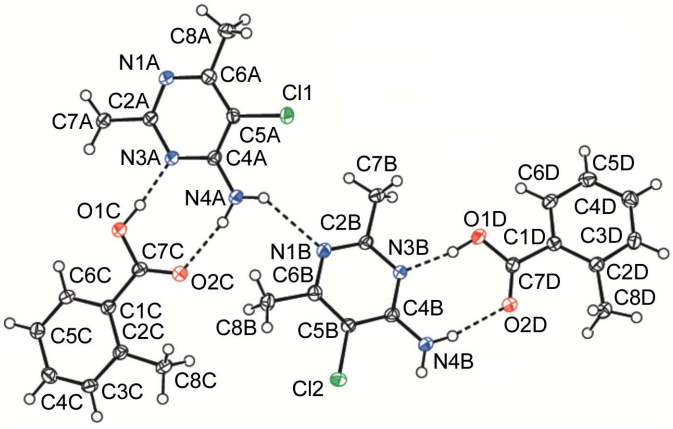


Figure 7
The asymmetric unit of cocrystal **7**, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Dashed lines represent hydrogen bonds.

The inversion-related stacked pyrimidines [pyrimidine–pyrimidine stacking interactions with a centroid-to-centroid (*Cg*1···*Cg*1) distance and a slip angle (the angle between the centroid vector and the normal to the plane) of 3.7050 (9) Å and 21.52°, respectively, for **1**, 3.6228 (13) Å and 21.69° for **2**, 3.7374 (16) Å and 24.71° for **3**, and 3.5182 (9) Å and 19.73° for **4**] are doubly bridged by the carboxyl groups *via* N—H···O and O—H···N hydrogen bonds to form a large cage-like

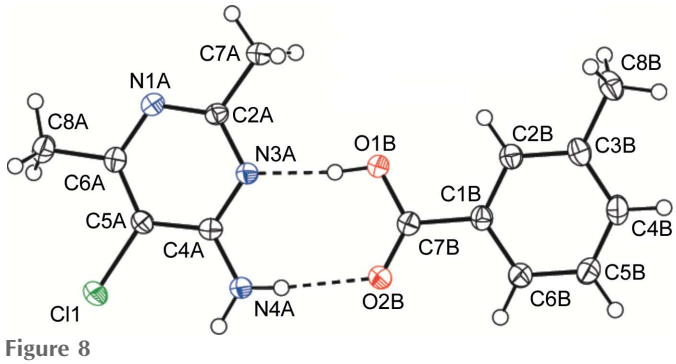


Figure 8
The asymmetric unit of cocrystal **8**, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Dashed lines represent hydrogen bonds.

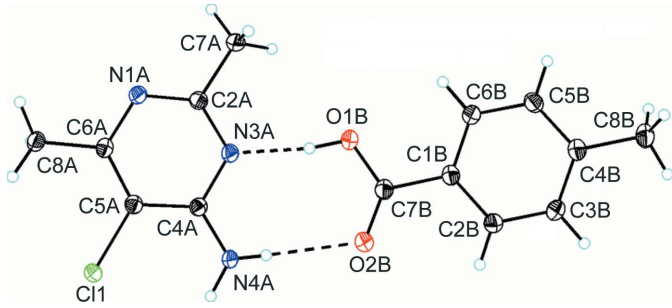


Figure 9
The asymmetric unit of cocrystal **9**, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Dashed lines represent hydrogen bonds.

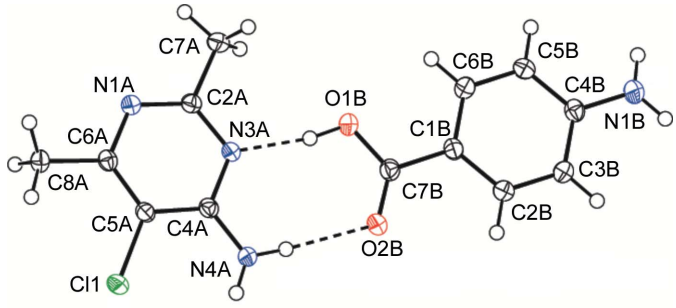


Figure 10
The asymmetric unit of cocrystal **10**, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Dashed lines represent hydrogen bonds.

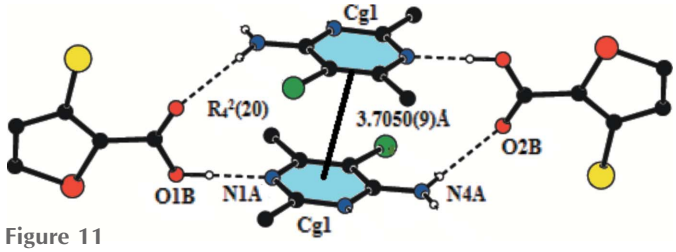


Figure 11
View of the large cage-like tetrameric unit in cocrystal **1**, with an $R_4^2(20)$ graph-set ring motif, and the π–π interactions between nearby pyrimidine moieties (*Cg*1···*Cg*1 centroid-to-centroid interaction; *Cg*1 is the centroid of the N1*A*/C1*A*/N3*A*/C4*A*–C6*A* ring). Dashed lined indicate intermolecular N—H···O and O—H···N hydrogen bonds. Generic centroid labels without symmetry codes have been used.

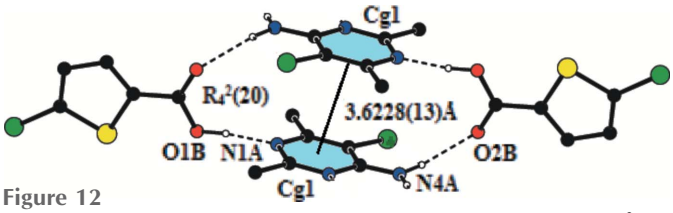


Figure 12
View of the large cage-like tetrameric unit in cocrystal **2**, with an $R_4^2(20)$ graph-set ring motif and π–π interactions between nearby pyrimidine moieties ($Cg1\cdots Cg1$ centroid-to-centroid interaction; $Cg1$ is the centroid of the N1*A*/C1*A*/N3*A*/C4*A*–C6*A* ring). Dashed lined indicate intermolecular N—H···O and O—H···N hydrogen bonds. Generic centroid labels without symmetry codes have been used.

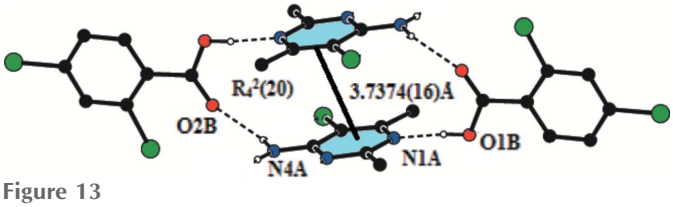


Figure 13
View of the large cage-like tetrameric unit in cocrystal **3**, with an $R_4^2(20)$ graph-set ring motif and π–π interactions between nearby pyrimidine moieties ($Cg1\cdots Cg1$ centroid-to-centroid interaction; $Cg1$ is the centroid of the N1*A*/C1*A*/N3*A*/C4*A*–C6*A* ring). Dashed lined indicate intermolecular N—H···O and O—H···N hydrogen bonds. Generic centroid labels without symmetry codes have been used.

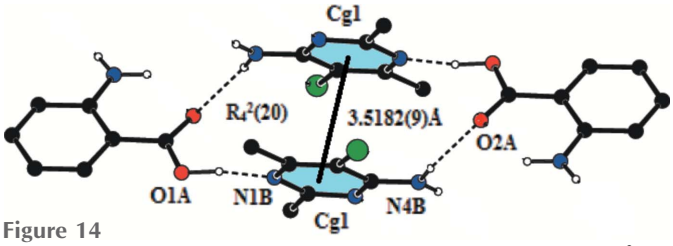


Figure 14
View of the large cage-like tetrameric unit in cocrystal **4**, with an $R_4^2(20)$ graph-set ring motif and π–π interactions between nearby pyrimidine moieties ($Cg1\cdots Cg1$ centroid-to-centroid interaction; $Cg1$ is the centroid of the N1*A*/C1*A*/N3*A*/C4*A*–C6*A* ring). Dashed lined indicate intermolecular N—H···O and O—H···N hydrogen bonds. Generic centroid labels without symmetry codes have been used.

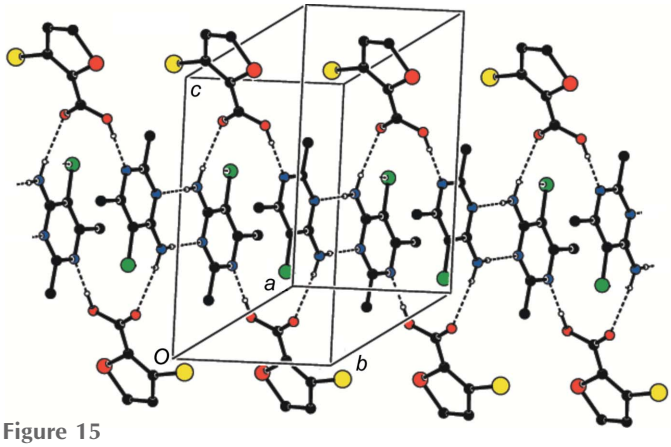


Figure 15
Crystal packing for cocrystal **1**, viewed along the *a* axis. Cage-like tetrameric units with $R_4^2(20)$ graph-set ring motifs are connected *via* base pairing through a pair of N—H···O and O—H···N hydrogen bonds (dashed lines), generating $R_2^2(8)$ ring motifs forming chains along (010). H atoms not involved in hydrogen bonding have been omitted for clarity.

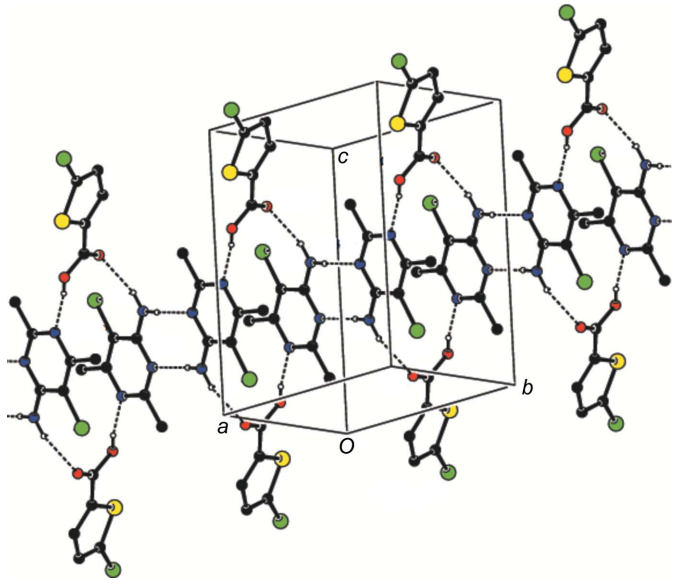


Figure 16
Crystal packing for cocrystal **2**, viewed along the *b* axis. Cage-like tetrameric units with $R_4^2(20)$ graph-set ring motifs are connected *via* base pairing through a pair of N—H···O and O—H···N hydrogen bonds (dashed lines), generating $R_2^2(8)$ ring motifs forming chains along (110). H atoms not involved in hydrogen bonding have been omitted for clarity.

tetrameric unit with an $R_4^2(20)$ graph-set ring motif (Figs. 11–14). The tetrameric units are further connected *via* base pairing through a pair of N—H···N hydrogen bonds, generating an $R_2^2(8)$ motif (supramolecular homosynthon) to form a single block (Figs. 15–18).

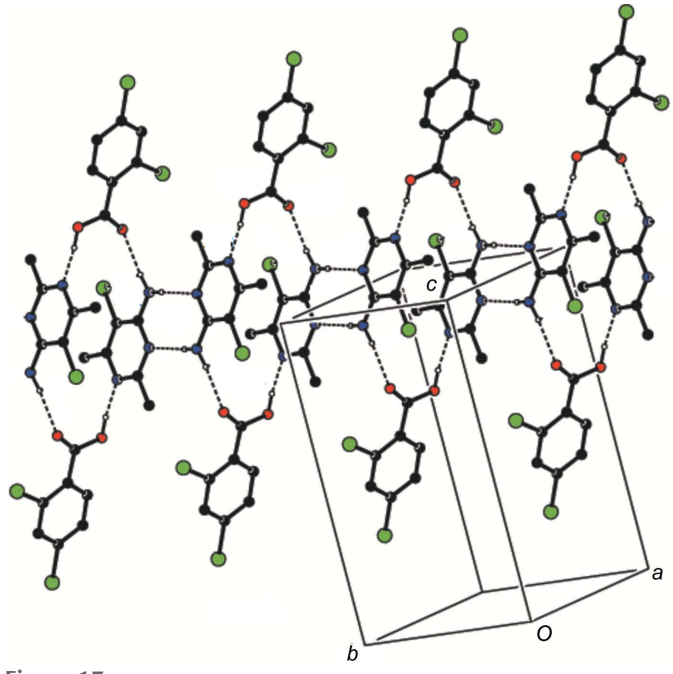


Figure 17
Crystal packing for cocrystal **3**, viewed along the *a* axis. Cage-like tetrameric units with $R_4^2(20)$ graph-set ring motifs are connected *via* base pairing through a pair of N—H···O and O—H···N hydrogen bonds (dashed lines), generating $R_2^2(8)$ ring motifs forming chains along (110). H atoms not involved in hydrogen bonding have been omitted for clarity.

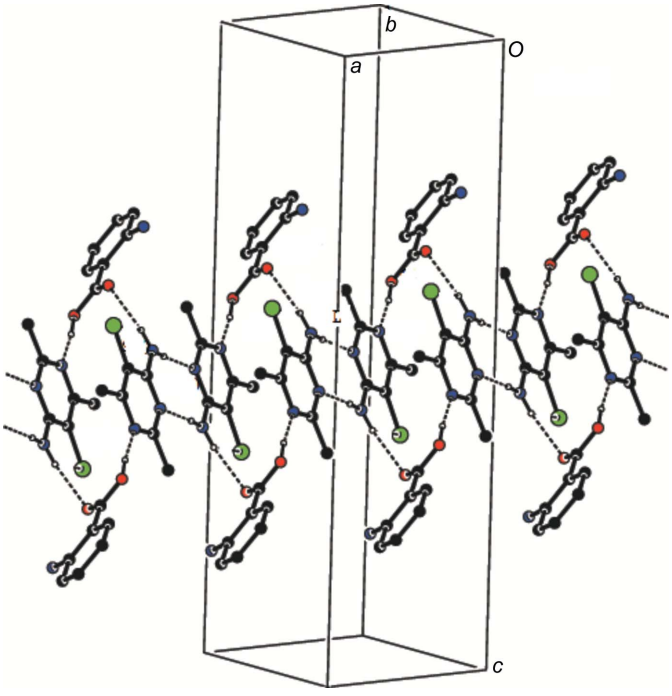


Figure 18
Crystal packing for cocrystal **4**, viewed along the *a* axis. Cage-like tetrameric units with $R_4^2(20)$ graph-set ring motifs are further connected *via* base pairing through a pair of N—H···O and O—H···N hydrogen bonds (dashed lines), generating $R_2^2(8)$ ring motifs forming chains along (110). H atoms not involved in hydrogen bonding have been omitted for clarity.

In the second series of cocrystals, *i.e.* **5**–**10**, the carboxyl group interacts with atom N3 and the adjacent 4-amino group of the corresponding pyrimidine moiety *via* O—H···N and N—H···O hydrogen bonds to generate the robust $R_2^2(8)$ supramolecular heterosynthon. These heterosynthons are further connected by N—H···N hydrogen-bond interactions

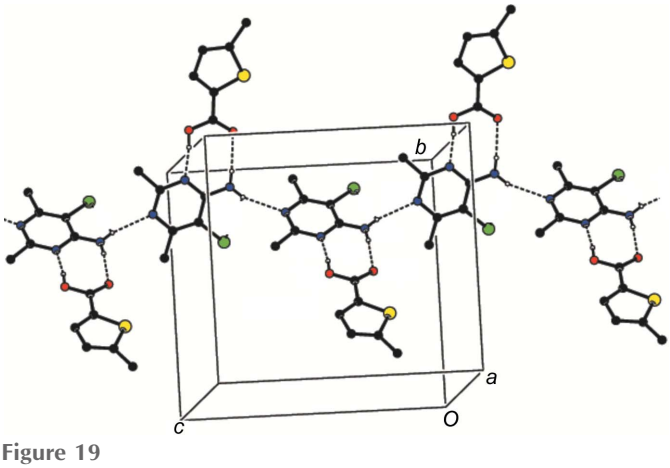


Figure 19
Crystal packing for cocrystal **5**, viewed along the *a* axis. Adjacent heterosynthons are connected by N—H···O and O—H···N hydrogen bonds (dashed lines), forming one-dimensional chains along (001). The heterosynthon occurs through a pair of N—H···N and O—H···N hydrogen bonds (dashed lines), generating $R_2^2(8)$ ring motifs directed along (010). H atoms not involved in hydrogen bonding have been omitted for clarity.

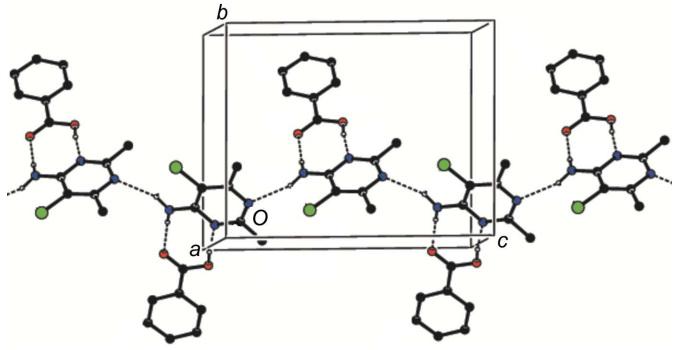


Figure 20
Crystal packing for cocrystal **6**, viewed along the *a* axis. Adjacent heterosynthons are connected by N—H···O hydrogen bonds (dashed lines), forming one-dimensional chains along (001). The heterosynthon occurs through a pair of N—H···N and O—H···N hydrogen bonds (dashed lines), generating $R_2^2(8)$ ring motifs directed along (010). H atoms not involved in hydrogen bonding have been omitted for clarity.

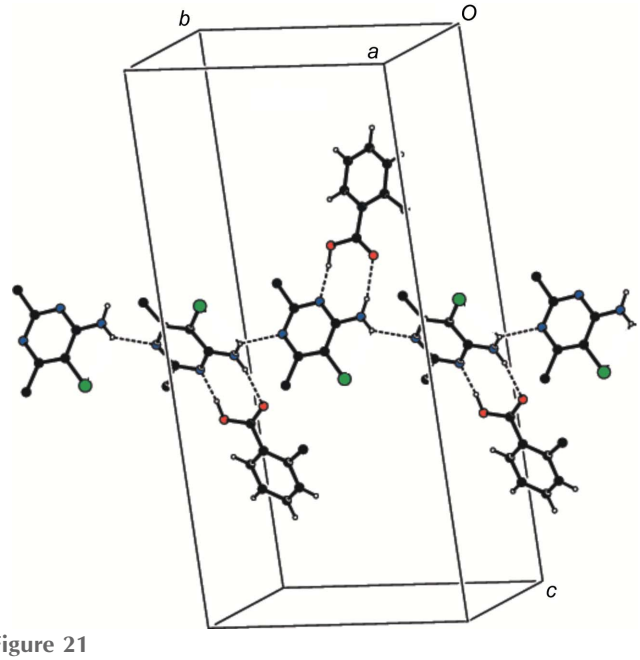


Figure 21
Crystal packing for cocrystal **7**, viewed along the *a* axis. Adjacent heterosynthons are connected by N—H···N hydrogen bonds (dashed lines), forming one-dimensional chains along (001). The heterosynthon occurs through a pair of N—H···O and O—H···N hydrogen bonds (dashed lines), generating $R_2^2(8)$ ring motifs directed along (010). H atoms not involved in hydrogen bonding have been omitted for clarity.

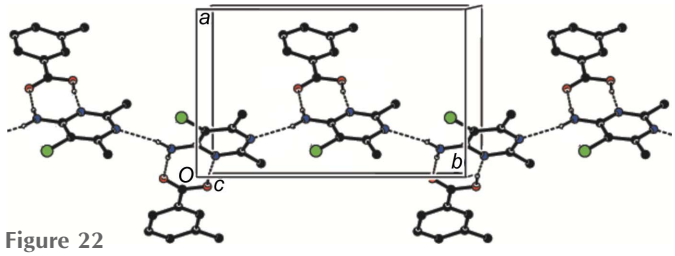


Figure 22
Crystal packing for cocrystal **8**, viewed along the *c* axis. Adjacent heterosynthons are connected by N—H···N hydrogen bonds (dashed lines), forming one-dimensional chains along (010). The heterosynthon occurs through a pair of N—H···O and O—H···N hydrogen bonds (dashed lines), generating $R_2^2(8)$ ring motifs directed along (100). H atoms not involved in hydrogen bonding have been omitted for clarity.

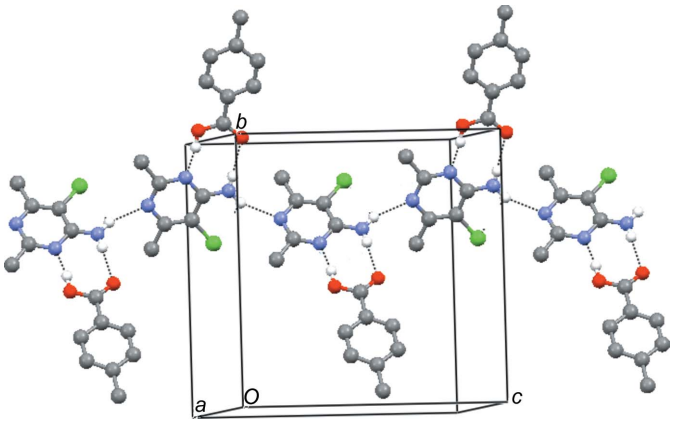


Figure 23
Crystal packing for cocrystal **9**, viewed along the *a* axis. Adjacent heterosynthons are connected by N—H···N hydrogen bonds (dashed lines), forming one-dimensional chains along (001). The heterosynthon occurs through a pair of N—H···O and O—H···N hydrogen bonds (dashed lines), generating $R_2^2(8)$ ring motifs directed along (010). H atoms not involved in hydrogen bonding have been omitted for clarity.

in a linear fashion to form a chain-like arrangement (Figs. 19–24). The occurrence of two series of cocrystals (depending upon the carboxyl –OH binding with N1 or N3) is reminiscent of the occurrence of two types of protonation (N1 or N3) in 6-amino-5-chloro-2,4-dimethylpyrimidin-1-ium 5-chloro-2-hydroxybenzoate, **I**, and 4-amino-5-chloro-2,6-dimethylpyrimidin-1-ium 5-chloro-2-hydroxybenzoate, **II** (Rajam *et al.*, 2017).

In the crystal structure of **1**, neighbouring blocks of the tetrameric units are connected by weak Br···Br halogen bonding [3.5693 (3) Å; Mukherjee & Desiraju, 2014; Tothadi *et al.*, 2013] and a C—H···Br hydrogen-bond interaction. In addition to this, π–π stacking interactions are present between the thiophene rings, with an observed interplanar distance of 3.504 Å, a centroid-to-centroid (*Cg*2···*Cg*2; *Cg*2 is the centroid of the S1*B*/C2*B*–C5*B* ring) distance of 3.6133 (10) Å and a slip angle (the angle between the centroid vector and the normal to the plane) of 14.15°, stabilizing the crystal structure and forming a three-dimensional superstructure (Fig. 25).

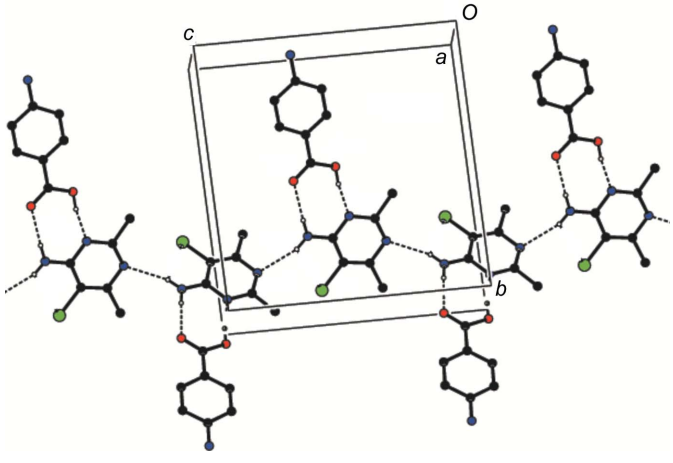


Figure 24
Crystal packing for cocrystal **10**, viewed along the *a* axis. Adjacent heterosynthons are connected by N—H···N hydrogen bonds (dashed lines), forming one-dimensional chains along (001). The heterosynthon occurs through a pair of N—H···O and O—H···N hydrogen bonds (dashed lines), generating $R_2^2(8)$ ring motifs directed along (010). H atoms not involved in hydrogen bonding have been omitted for clarity.

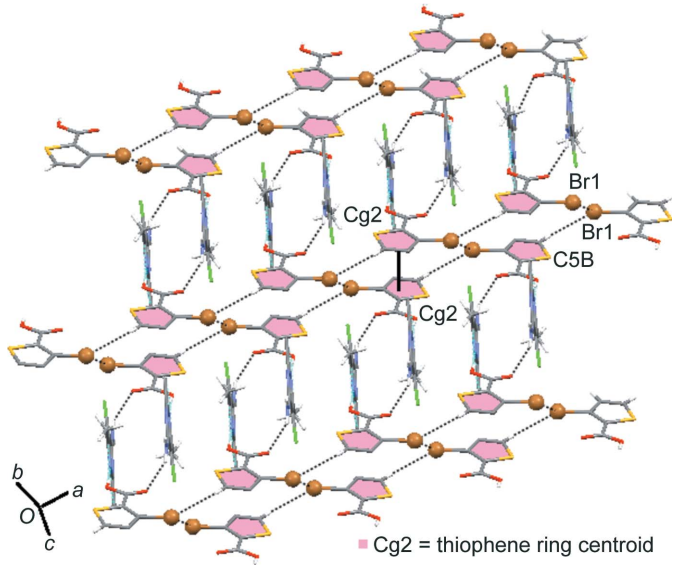


Figure 25
An overall packing view of cocrystal **1** containing large cage-like tetrameric units with $R_4^2(20)$ graph-set ring motifs derived from intermolecular N—H···O and O—H···N hydrogen bonds (dashed lines) and π–π interactions between nearby pyrimidine moieties. Neighbouring blocks are connected by weak Br(acid)···Br(acid), C—H···Br and π(acid)–π(acid) (*Cg*2···*Cg*2) stacking of thiophene (pink) moieties. H atoms not involved in hydrogen bonding have been omitted for clarity. Generic atom and centroid labels without symmetry codes are shown

For the crystal structure of **2**, neighbouring blocks of the tetrameric units are connected by weak Cl···Cl halogen bonds [3.3736 (9) Å; Mukherjee & Desiraju, 2014; Tothadi *et al.*, 2013] and C—H···Cl hydrogen-bond interactions. In addition to this, π–π interactions are observed between the thiophene rings, with an observed interplanar distance of 3.493 Å, a centroid-to-centroid (*Cg*2···*Cg*2; *Cg*2 is the centroid of the S1*B*/C2*B*–C5*B* ring) distance of 3.8466 (14) Å and a slip angle of 24.77° (Fig. 26).

In the crystal structure of **3**, neighbouring blocks of the tetrameric units are connected by a Cl···Cl halogen bond [3.4967 (9) Å; Mukherjee & Desiraju, 2014; Tothadi *et al.*, 2013]. In addition to this, π–π stacking interactions between the benzene rings, with an observed interplanar distance of 3.477 Å, a centroid-to-centroid (*Cg*2···*Cg*2; *Cg*2 is the centroid of the C1*B*–C6*B* ring) distance of 3.8815 (17) Å and a slip angle of 26.39°, are also present to stabilize the supramolecular architecture (Fig. 27).

In the crystal structure of **4**, neighbouring blocks of the tetrameric units are connected by aromatic C—H···π interactions, with the distance from the proton to the acceptor ring, *i.e.* (C4*B*—)H4*BA*···*Cg*2, being 2.66 Å (*Cg*2 is the centroid of the C1*B*–C6*B* ring), forming a three-dimensional superstructure (Fig. 28).

In the crystal structure of **5**, two inversion-related heterotetramers are connected through N—H···N hydrogen bonds

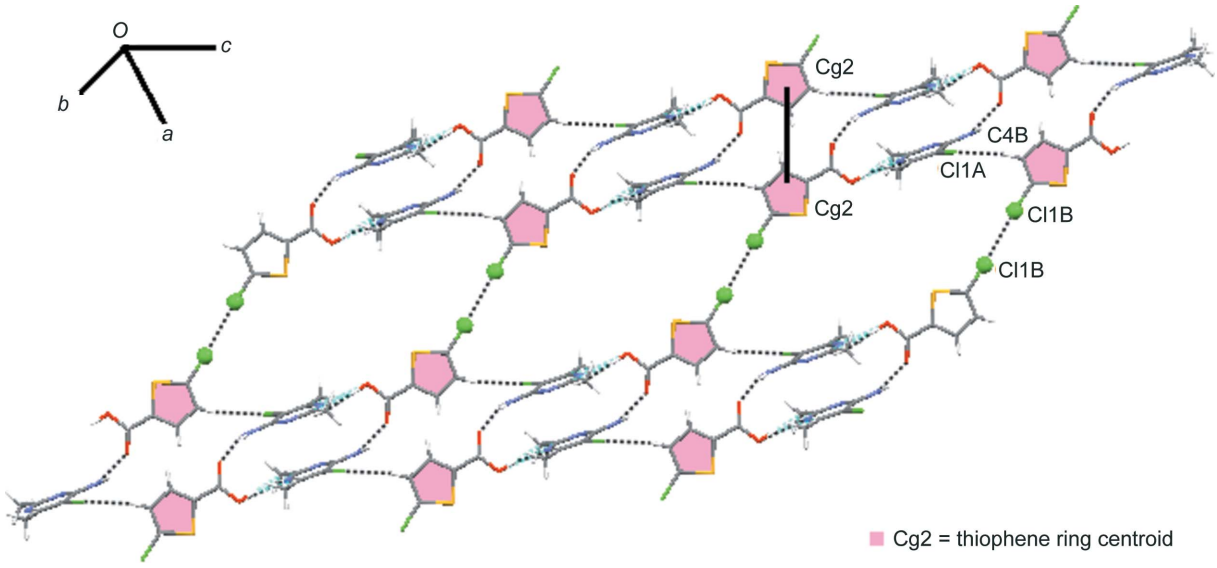


Figure 26
An overall packing view of cocrystal **2** containing large cage-like tetrameric units with $R_4^2(20)$ graph-set ring motifs derived from intermolecular N—H···O and O—H···N hydrogen bonds (dashed lines) and π–π interactions between nearby pyrimidine moieties. Neighbouring blocks are connected by weak Cl(acid)···Cl(acid), C—H···Cl and π(acid)–π(acid) (*Cg*2···*Cg*2) stacking of thiophene (pink) moieties. H atoms not involved in hydrogen bonding have been omitted for clarity. Generic atom and centroid labels without symmetry codes are shown

and a Cl···O halogen bond (3.2022 Å; Mukherjee & Desiraju, 2014; Lu *et al.*, 2009) to form a cyclic ring motif. In addition to this, π–π stacking interactions between the pyrimidine and the acid ring, with an observed interplanar distance of 3.520 Å, a centroid-to-centroid (*Cg*1···*Cg*2; *Cg*1 is the centroid of the N1*A*/C2*A*/N3*A*/C4*A*–C6*A* ring and *Cg*2 is the centroid of the S1*B*/C1*B*–C5*B* ring) distance of 3.8002 (16) Å and a slip angle of 21.06°, are also present to stabilize the crystal structure (Fig. 29).

In the crystal structure of **6**, the hydrogen-bonded ring is formed by the interconnection of two inversion-related heterotetramers through N—H···N hydrogen bonds and a Cl···O halogen bond (2.9926 Å; Mukherjee & Desiraju, 2014; Lu *et al.*, 2009) (Fig. 30).

In the crystal structure of **7**, two of the heterotetramers are connected through N—H···N hydrogen bonds and a Cl···O halogen bond [3.121 (18) Å; Mukherjee & Desiraju, 2014; Lu *et al.*, 2009] to form a cyclic ring. Two distinct π–π stacking interactions between pyrimidine/pyrimidine [with an observed interplanar distance of 3.429 Å, a centroid-to-centroid (*Cg*1···*Cg*2; *Cg*1 is the centroid of the N1*A*/C2*A*/N3*A*/C4*A*–C6*A* ring and *Cg*2 is the centroid of the N1*B*/C2*B*/N3*B*/C4*B*–C6*B* ring) distance of 3.6946 (15) Å and slip angle of 21.87°] and acid/acid [with an observed interplanar distance of

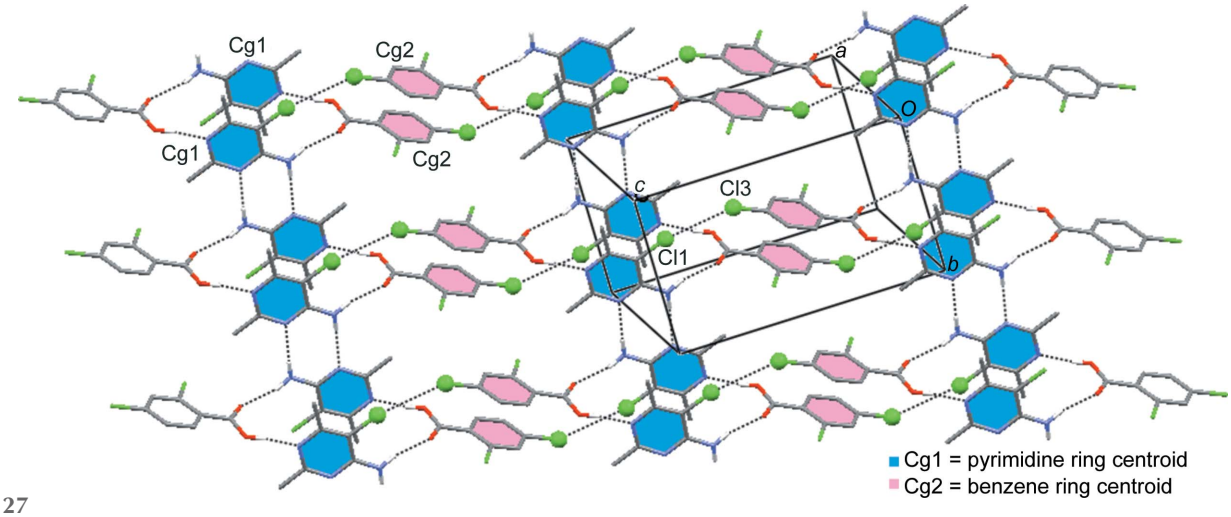


Figure 27
An overall packing view of cocrystal **3** containing large cage-like tetrameric units with $R_4^2(20)$ graph-set ring motifs derived from intermolecular N—H···O and O—H···N hydrogen bonds (dashed lines) and π–π interactions, *i.e.* *Cg*1···*Cg*1 centroid-to-centroid interactions (blue), of nearby pyrimidine moieties. Neighbouring blocks are further connected by weak Cl(pyrimidine)···Cl(acid), C—H···Cl and π(acid)–π(acid) (*Cg*2···*Cg*2) stacking of phenyl (pink) moieties. H atoms not involved in hydrogen bonding have been omitted for clarity. Generic atom and centroid labels without symmetry codes are shown

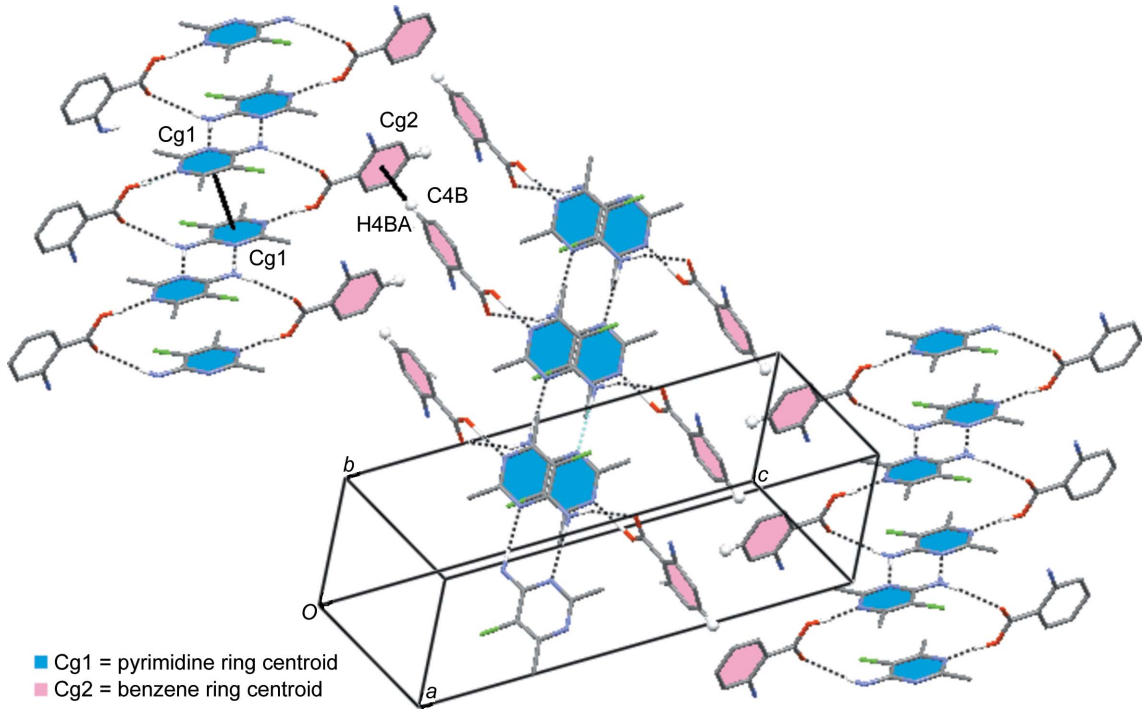


Figure 28
An overall packing view of cocrystal **4** containing large cage-like tetrameric units with $R_4^2(20)$ graph-set ring motifs derived from intermolecular N—H···O and O—H···N hydrogen bonds (dashed lines) and π–π interactions, *i.e.* *Cg*1···*Cg*1 centroid-to-centroid interactions (blue), of nearby pyrimidine moieties. Neighbouring blocks are connected by weak *Cg*2···π interactions (C—H···*Cg*2, pink) of nearby phenyl moieties (dashed lines) contribute to form a three-dimensional superstructure. H atoms not involved in hydrogen bonding have been omitted for clarity. Generic atom and centroid labels without symmetry codes are shown

3.353 Å, a centroid-to-centroid (*Cg*3···*Cg*4; *Cg*3 is the centroid of the C1*C*–C6*C* ring and *Cg*4 is the centroid of the C1*D*–C6*D* ring) distance of 3.6319 (17) Å and a slip angle of 22.61°] are also observed (Fig. 31).

In the crystal structure of **8**, two of the inversion-related heterotetramers are connected through N—H···N and C—H···O hydrogen-bond interactions to form a cyclic ring motif. π–π stacking interactions between the pyrimidine rings, with an observed interplanar distance of 3.508 Å, a centroid-to-centroid (*Cg*1···*Cg*1; *Cg*1 is the centroid of the N1*A*/C2*A*/

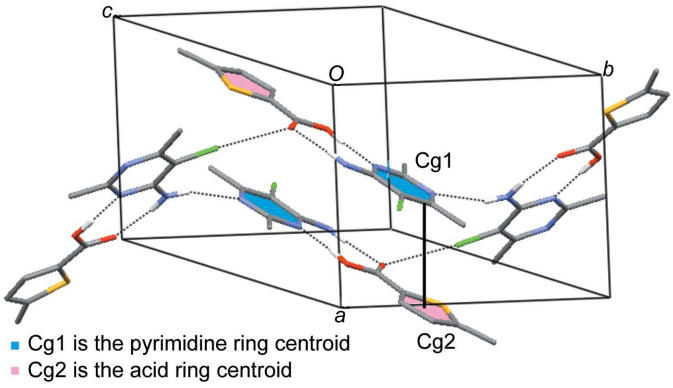


Figure 29
An overall packing view of cocrystal **5**, viewed along the *c* axis, containing large cage-like hydrogen bonded units with $R_4^4(24)$ graph-set ring motifs derived from intermolecular N—H···N and O—H···N hydrogen bonds (dashed lines) connecting the pyrimidine (blue) and thiophene (pink) rings and C—Cl···O intermolecular interactions which are displayed. Additional weak π–π *Cg*1(pyrimidine)···*Cg*2(thiophene) intermolecular interactions are also present forming a two-dimensional network along (001). H atoms not involved in hydrogen bonding have been omitted for clarity

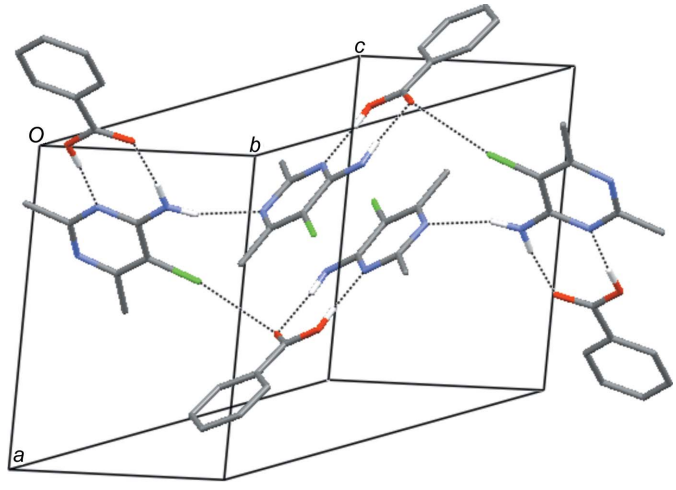


Figure 30
An overall packing view of cocrystal **6**, viewed along the *c* axis, containing large cage-like hydrogen bonded units with $R_4^4(24)$ graph-set ring motifs derived from intermolecular N—H···N and O—H···N hydrogen bonds (dashed lines) connecting the pyrimidine and phenyl rings and C—Cl···O intermolecular interactions which are displayed. Additional weak π–π *Cg*1(pyrimidine)···*Cg*2(phenyl) intermolecular interactions (not indicated) are also present forming a two-dimensional network along (001). H atoms not involved in hydrogen bonding have been omitted for clarity

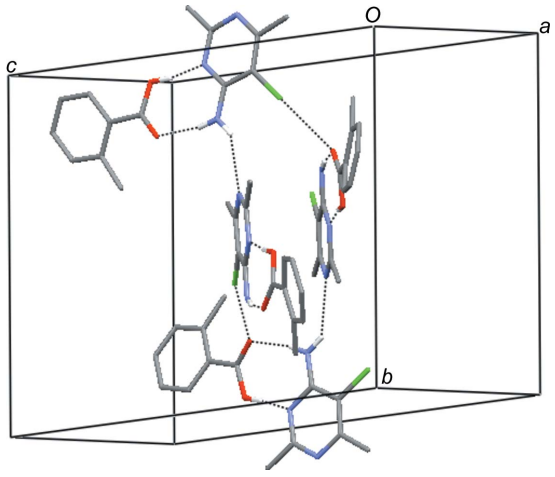


Figure 31
An overall packing view of cocrystal **7**, viewed along the *c* axis containing large cage-like hydrogen bonded units with $R_4^4(20)$ graph-set ring motifs derived from intermolecular N—H···N and O—H···N hydrogen bonds (dashed lines) connecting the pyrimidine and phenyl rings and C—Cl···O intermolecular interactions which are displayed. Additional weak π–π *Cg*(pyrimidine)···*Cg*2(phenyl) intermolecular interactions (not indicated) are also present forming a two-dimensional network along (001). H atoms not involved in hydrogen bonding have been omitted for clarity

N3*A*/C4*A*–C6*A* ring) distance of 3.6145 (7) Å and a slip angle of 13.91°, are also observed (Fig. 32).

In the crystal structure of **9**, two inversion-related heterotetramers are connected through N—H···N and C—H···O hydrogen-bond interactions to form a cyclic ring motif. In addition to this, π–π stacking interactions between the pyrimidine moiety and the acid ring, with an observed interplanar distance of 3.384 Å, a centroid-to-centroid (*Cg*1···*Cg*2; *Cg*1 is the centroid of the N1*A*/C2*A*/N3*A*/C4*A*–C6*A* ring and *Cg*2 is the centroid of the C1*B*–C6*B* ring) distance of 3.6186 Å and a slip angle of 18.94° are also present to help stabilize the crystal structure (Fig. 33).

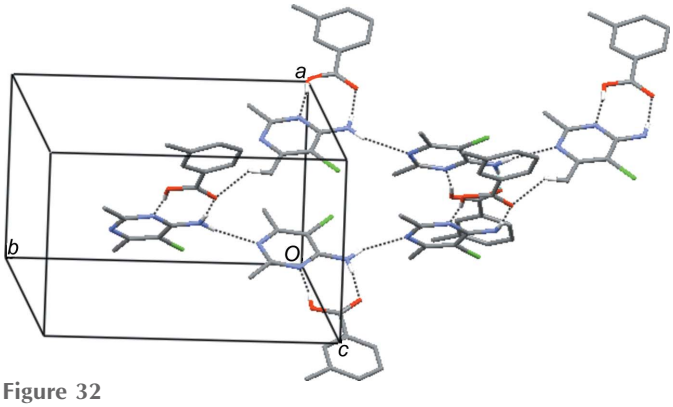


Figure 32
An overall packing view of cocrystal **8**, viewed along the *c* axis, containing large cage-like hydrogen-bonded units with $R_8^8(34)$ graph-set ring motifs derived from intermolecular N—H···N and O—H···N hydrogen bonds (dashed lines) connecting the pyrimidine and phenyl rings and N—H···N intermolecular interactions which are displayed. Additional weak π–π *Cg*1(pyrimidine)···*Cg*1(pyrimidine) intermolecular interactions (not indicated) are also present forming a two-dimensional network along (010). H atoms not involved in hydrogen bonding have been omitted for clarity

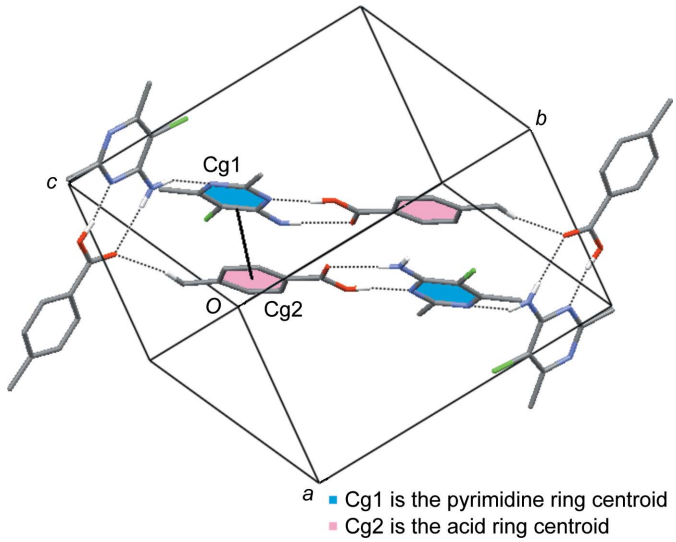


Figure 33
An overall packing view of cocrystal **9**, viewed along the *c* axis containing large cage-like hydrogen bonded units with $R_8^8(34)$ graph-set ring motifs derived from intermolecular N—H···N and O—H···N hydrogen bonds (dashed lines) connecting the pyrimidine and phenyl rings and N—H···N intermolecular interactions which are displayed. Additional weak π–π *Cg*1(pyrimidine)···*Cg*2(phenyl) intermolecular interactions are also present forming a two-dimensional network along (111). H atoms not involved in hydrogen bonding have been omitted for clarity

In the crystal structure of **10**, two of the inversion-related heterotetramers are connected through N—H···N and N—H···O hydrogen-bond interactions to form a cyclic ring motif. In addition to this, π–π stacking interactions between the rings of the pyrimidine and acid molecules are observed, with an

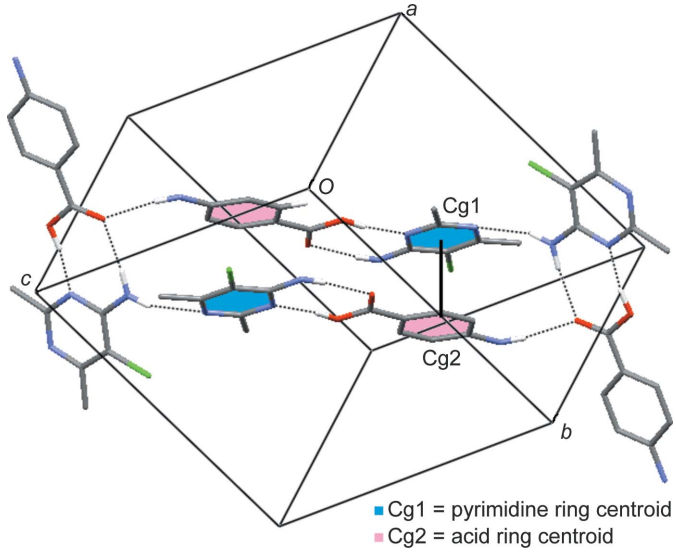


Figure 34
An overall packing view of cocrystal **10**, viewed along the *c* axis containing large cage-like hydrogen-bonded units with $R_8^8(34)$ graph-set ring motifs derived from intermolecular N—H···N and O—H···N hydrogen bonds (dashed lines) connecting the pyrimidine and phenyl rings and N—H···N intermolecular interactions which are displayed. Additional weak π–π *Cg*1(pyrimidine)···*Cg*2(phenyl) intermolecular interactions are also present forming a two-dimensional network along (111). H atoms not involved in hydrogen bonding have been omitted for clarity

interplanar distance of 3.464 Å, a centroid-to-centroid ($Cg1\cdots Cg2$; $Cg1$ is the centroid of the N1A/C2A/N3A/C4A–C6A ring and $Cg2$ is the centroid of the C1B–C6B ring) distance of 3.5283 (8) Å and a slip angle of 9.65°, are also found to help stabilize the crystal structure (Fig. 34).

It is very interesting to observe two series of cocrystals involving 4-amino-5-chloro-2,6-dimethylpyrimidine and carboxylic acids. In one series of cocrystals, the carboxyl hydroxy group (–OH) is hydrogen bonded to atom N1 (O—H···N1) of the corresponding pyrimidine ring (single point supramolecular synthon). In the other series, the carboxyl group interacts with atom N3 and the adjacent 4-amino group of the corresponding pyrimidine *via* O—H···N and N—H···O hydrogen bonds to generate a robust $R_2^2(8)$ supramolecular heterosynthon. This is similarly reminiscent of two types of protonation, at N1 or N3 of 4-amino-5-chloro-2,6-dimethylpyrimidine, reported recently (Rajam *et al.*, 2017). Further studies may reveal whether each of the cocrystals of one series will have a polymorphic form corresponding to the other series of cocrystals, similar to the cation tautomerism reported for this type of pyrimidine interaction (Rajam *et al.*, 2017).

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supporting information

Acta Cryst. (2018). C**74**, 1007-1019 [https://doi.org/10.1107/S2053229618009154]

Design of two series of 1:1 cocrystals involving 4-amino-5-chloro-2,6-dimethylpyrimidine and carboxylic acids

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Computing details

Data collection: *APEX2* (Bruker, 2014) for COCRYSTAL-1, COCRYSTAL-2, COCRYSTAL-5; *CrysAlis PRO* (Agilent, 2014) for COCRYSTAL-3, COCRYSTAL-6, COCRYSTAL-7, COCRYSTAL-8, COCRYSTAL-9, COCRYSTAL-10; *CrysAlis PRO* (Oxford Diffraction, 2011) for COCRYSTAL-4. Cell refinement: *SAINT* (Bruker, 2014) for COCRYSTAL-1, COCRYSTAL-2; *CrysAlis PRO* (Agilent, 2014) for COCRYSTAL-3, COCRYSTAL-6, COCRYSTAL-7, COCRYSTAL-8, COCRYSTAL-9, COCRYSTAL-10; *CrysAlis PRO* (Oxford Diffraction, 2011) for COCRYSTAL-4; *SAINT* (Bruker, 2013) for COCRYSTAL-5. Data reduction: *SAINT* (Bruker, 2014) for COCRYSTAL-1, COCRYSTAL-2; *CrysAlis PRO* (Agilent, 2014) for COCRYSTAL-3, COCRYSTAL-6, COCRYSTAL-7, COCRYSTAL-8, COCRYSTAL-9, COCRYSTAL-10; *CrysAlis PRO* (Oxford Diffraction, 2011) for COCRYSTAL-4; *SAINT* (Bruker, 2013) for COCRYSTAL-5. Program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008) for COCRYSTAL-1, COCRYSTAL-2, COCRYSTAL-5; SHELXT (Sheldrick, 2015a) for COCRYSTAL-3, COCRYSTAL-4, COCRYSTAL-6, COCRYSTAL-7, COCRYSTAL-8, COCRYSTAL-9, COCRYSTAL-10. Program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b) for COCRYSTAL-1, COCRYSTAL-2; *SHELXL2014* (Sheldrick, 2015b) for COCRYSTAL-3, COCRYSTAL-4, COCRYSTAL-6, COCRYSTAL-7, COCRYSTAL-8, COCRYSTAL-9, COCRYSTAL-10; *SHELXL2014* (Sheldrick, 2015b) and shelXle (Hübschle *et al.*, 2011) for COCRYSTAL-5. Molecular graphics: *SHELXTL* (Sheldrick, 2008) for COCRYSTAL-1, COCRYSTAL-2, COCRYSTAL-3, COCRYSTAL-4, COCRYSTAL-7, COCRYSTAL-8, COCRYSTAL-9, COCRYSTAL-10; SHELXT (Sheldrick, 2008) for COCRYSTAL-6. Software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) for COCRYSTAL-1, COCRYSTAL-2, COCRYSTAL-3, COCRYSTAL-4, COCRYSTAL-7, COCRYSTAL-8, COCRYSTAL-9, COCRYSTAL-10; SHELXT (Sheldrick, 2008) for COCRYSTAL-6.

4-Amino-5-chloro-2,6-dimethylpyrimidine–3-bromothiophene-2-carboxylic acid (1/1) (COCRYSTAL-1)

Crystal data

$C_5H_3BrO_2S·C_6H_8ClN_3$
M_r = 364.65
Triclinic, $P\overline{1}$
a = 7.5237 (4) Å
b = 7.5739 (4) Å
c = 12.5089 (7) Å
α = 79.629 (2)°
β = 79.596 (2)°
γ = 75.895 (2)°
V = 673.00 (6) Å^3
Z = 2
$F(000)$ = 364
D_x = 1.799 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9311 reflections
θ = 2.8–33.2°
μ = 3.41 mm^{-1}
T = 100 K
Block, colourless
0.31 × 0.27 × 0.21 mm

Data collection

Bruker D8 Quest CMOS diffractometer
Radiation source: I-mu-S microsource X-ray tube
ω and phi scans
Absorption correction: multi-scan (APEX2; Bruker, 2014)
T_{min} = 0.539, T_{max} = 0.747
13063 measured reflections
5103 independent reflections
4471 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 33.2°, θ_{min} = 2.8°
h = −11→10
k = −11→11
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.070
S = 1.04
5103 reflections
187 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.010P)^2 + 0.8813P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Br1	0.17359 (2)	−0.20786 (2)	0.99807 (2)	0.01468 (5)	
S1	0.71218 (6)	−0.09607 (6)	0.83962 (4)	0.01414 (9)	
O1B	0.4649 (2)	0.1721 (2)	0.71276 (12)	0.0203 (3)	
H1A	0.396 (5)	0.264 (5)	0.673 (3)	0.050 (10)*	
O2B	0.1948 (2)	0.1035 (2)	0.79633 (13)	0.0221 (3)	
C1B	0.3626 (3)	0.0767 (2)	0.78633 (15)	0.0134 (3)	
C2B	0.4747 (2)	−0.0686 (2)	0.85783 (14)	0.0113 (3)	
C3B	0.4191 (2)	−0.1903 (2)	0.94601 (15)	0.0108 (3)	
C4B	0.5662 (2)	−0.3038 (2)	0.99870 (15)	0.0131 (3)	
H4AA	0.550993	−0.393948	1.061103	0.016*	
C5B	0.7327 (3)	−0.2678 (2)	0.94879 (16)	0.0156 (3)	
H5AA	0.847630	−0.331186	0.972153	0.019*	
Cl1	0.20623 (6)	0.53889 (6)	0.26918 (4)	0.01714 (9)	
N1A	0.2875 (2)	0.4395 (2)	0.58151 (13)	0.0135 (3)	
C1A	0.2123 (2)	0.6060 (2)	0.61071 (15)	0.0128 (3)	
N3A	0.1304 (2)	0.7519 (2)	0.54593 (13)	0.0127 (3)	
N4A	0.0334 (2)	0.8728 (2)	0.37794 (14)	0.0146 (3)	
H4B1	−0.013 (4)	0.970 (4)	0.401 (2)	0.027 (7)*	
H4B2	0.012 (4)	0.856 (4)	0.318 (2)	0.027 (7)*	
C4A	0.1219 (2)	0.7307 (2)	0.44175 (14)	0.0111 (3)	

C5A	0.2057 (2)	0.5596 (2)	0.40456 (14)	0.0117 (3)	
C6A	0.2853 (2)	0.4153 (2)	0.47652 (15)	0.0129 (3)	
C7A	0.2190 (3)	0.6288 (3)	0.72665 (16)	0.0184 (4)	
H7BA	0.346202	0.583683	0.742949	0.028*	
H7BB	0.137498	0.558307	0.777376	0.028*	
H7BC	0.177617	0.759176	0.735254	0.028*	
C8A	0.3708 (3)	0.2269 (3)	0.44675 (17)	0.0193 (4)	
H8B1	0.413316	0.144726	0.511493	0.029*	0.50 (3)
H8B2	0.476348	0.233326	0.388531	0.029*	0.50 (3)
H8B3	0.278688	0.179407	0.420768	0.029*	0.50 (3)
H8B4	0.376237	0.229615	0.367619	0.029*	0.50 (3)
H8B5	0.295740	0.140367	0.486933	0.029*	0.50 (3)
H8B6	0.496375	0.187476	0.466240	0.029*	0.50 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01179 (8)	0.01544 (8)	0.01657 (9)	−0.00349 (6)	−0.00291 (6)	−0.00006 (6)
S1	0.01211 (18)	0.01347 (19)	0.0168 (2)	−0.00285 (14)	−0.00211 (15)	−0.00203 (15)
O1B	0.0187 (6)	0.0178 (6)	0.0202 (7)	−0.0021 (5)	−0.0034 (5)	0.0064 (5)
O2B	0.0174 (6)	0.0246 (7)	0.0219 (8)	−0.0032 (5)	−0.0092 (6)	0.0072 (6)
C1B	0.0168 (8)	0.0131 (7)	0.0107 (8)	−0.0022 (6)	−0.0044 (6)	−0.0018 (6)
C2B	0.0122 (7)	0.0107 (7)	0.0115 (8)	−0.0014 (6)	−0.0042 (6)	−0.0018 (6)
C3B	0.0104 (7)	0.0098 (7)	0.0131 (8)	−0.0016 (5)	−0.0033 (6)	−0.0034 (6)
C4B	0.0161 (7)	0.0106 (7)	0.0139 (8)	−0.0024 (6)	−0.0075 (6)	−0.0002 (6)
C5B	0.0147 (7)	0.0130 (8)	0.0196 (9)	−0.0008 (6)	−0.0076 (7)	−0.0019 (6)
Cl1	0.0222 (2)	0.0184 (2)	0.01073 (19)	−0.00160 (16)	−0.00411 (16)	−0.00395 (15)
N1A	0.0160 (7)	0.0110 (6)	0.0125 (7)	−0.0013 (5)	−0.0039 (5)	0.0004 (5)
C1A	0.0138 (7)	0.0125 (7)	0.0118 (8)	−0.0030 (6)	−0.0034 (6)	0.0006 (6)
N3A	0.0156 (7)	0.0112 (6)	0.0111 (7)	−0.0026 (5)	−0.0035 (5)	−0.0004 (5)
N4A	0.0205 (7)	0.0100 (7)	0.0123 (7)	0.0002 (6)	−0.0063 (6)	−0.0002 (5)
C4A	0.0112 (7)	0.0110 (7)	0.0111 (7)	−0.0030 (5)	−0.0019 (6)	−0.0005 (6)
C5A	0.0146 (7)	0.0115 (7)	0.0090 (7)	−0.0025 (6)	−0.0023 (6)	−0.0012 (5)
C6A	0.0131 (7)	0.0118 (7)	0.0130 (8)	−0.0029 (6)	−0.0012 (6)	−0.0001 (6)
C7A	0.0242 (9)	0.0207 (9)	0.0106 (8)	−0.0035 (7)	−0.0062 (7)	−0.0012 (6)
C8A	0.0225 (9)	0.0122 (8)	0.0203 (9)	0.0017 (7)	−0.0032 (7)	−0.0023 (7)

Geometric parameters (Å, º)

Br1—C3B	1.8729 (17)	C1A—N3A	1.335 (2)
Br1—Br1^{i}	3.5693 (4)	C1A—C7A	1.502 (3)
Br1—Cl1^{ii}	3.6014 (5)	N3A—C4A	1.356 (2)
Br1—S1^{iii}	3.6656 (5)	N4A—C4A	1.331 (2)
S1—C5B	1.7083 (19)	N4A—H4B1	0.81 (3)
S1—C2B	1.7253 (17)	N4A—H4B2	0.83 (3)
O1B—C1B	1.318 (2)	C4A—C5A	1.416 (2)
O1B—H1A	0.89 (3)	C5A—C6A	1.373 (2)
O2B—C1B	1.216 (2)	C6A—C8A	1.499 (3)

C1B—C2B	1.479 (2)	C7A—H7BA	0.9800
C2B—C3B	1.377 (2)	C7A—H7BB	0.9800
C3B—C4B	1.412 (2)	C7A—H7BC	0.9800
C4B—C5B	1.362 (3)	C8A—H8B1	0.9800
C4B—H4AA	0.9500	C8A—H8B2	0.9800
C5B—H5AA	0.9500	C8A—H8B3	0.9800
Cl1—C5A	1.7276 (18)	C8A—H8B4	0.9800
N1A—C1A	1.337 (2)	C8A—H8B5	0.9800
N1A—C6A	1.362 (2)	C8A—H8B6	0.9800

C3B—Br1—Br1^{i}	118.11 (5)	C4A—N4A—H4B2	118.9 (19)
C3B—Br1—Cl1^{ii}	102.47 (5)	H4B1—N4A—H4B2	120 (3)
Br1^{i}—Br1—Cl1^{ii}	111.923 (11)	N4A—C4A—N3A	118.32 (16)
C3B—Br1—S1^{iii}	73.14 (5)	N4A—C4A—C5A	122.24 (16)
Br1^{i}—Br1—S1^{iii}	69.809 (10)	N3A—C4A—C5A	119.44 (15)
Cl1^{ii}—Br1—S1^{iii}	73.552 (12)	C6A—C5A—C4A	119.30 (16)
C5B—S1—C2B	91.90 (9)	C6A—C5A—Cl1	121.77 (14)
C1B—O1B—H1A	112 (2)	C4A—C5A—Cl1	118.93 (13)
O2B—C1B—O1B	124.83 (17)	N1A—C6A—C5A	119.82 (16)
O2B—C1B—C2B	122.74 (17)	N1A—C6A—C8A	116.65 (16)
O1B—C1B—C2B	112.43 (15)	C5A—C6A—C8A	123.52 (17)
C3B—C2B—C1B	129.82 (16)	C1A—C7A—H7BA	109.5
C3B—C2B—S1	110.12 (12)	C1A—C7A—H7BB	109.5
C1B—C2B—S1	119.99 (13)	H7BA—C7A—H7BB	109.5
C2B—C3B—C4B	113.85 (15)	C1A—C7A—H7BC	109.5
C2B—C3B—Br1	125.30 (13)	H7BA—C7A—H7BC	109.5
C4B—C3B—Br1	120.84 (13)	H7BB—C7A—H7BC	109.5
C5B—C4B—C3B	111.48 (16)	C6A—C8A—H8B1	109.5
C5B—C4B—H4AA	124.3	C6A—C8A—H8B2	109.5
C3B—C4B—H4AA	124.3	H8B1—C8A—H8B2	109.5
C4B—C5B—S1	112.65 (13)	C6A—C8A—H8B3	109.5
C4B—C5B—H5AA	123.7	H8B1—C8A—H8B3	109.5
S1—C5B—H5AA	123.7	H8B2—C8A—H8B3	109.5
C1A—N1A—C6A	118.14 (15)	C6A—C8A—H8B4	109.5
N3A—C1A—N1A	125.43 (17)	C6A—C8A—H8B5	109.5
N3A—C1A—C7A	117.73 (16)	H8B4—C8A—H8B5	109.5
N1A—C1A—C7A	116.83 (15)	C6A—C8A—H8B6	109.5
C1A—N3A—C4A	117.78 (15)	H8B4—C8A—H8B6	109.5
C4A—N4A—H4B1	121 (2)	H8B5—C8A—H8B6	109.5

O2B—C1B—C2B—C3B	−2.5 (3)	C3B—C4B—C5B—S1	0.7 (2)
O1B—C1B—C2B—C3B	177.09 (18)	C2B—S1—C5B—C4B	−0.41 (15)
O2B—C1B—C2B—S1	−179.15 (15)	C6A—N1A—C1A—N3A	1.6 (3)
O1B—C1B—C2B—S1	0.4 (2)	C6A—N1A—C1A—C7A	−179.29 (16)
C5B—S1—C2B—C3B	0.04 (14)	N1A—C1A—N3A—C4A	0.1 (3)
C5B—S1—C2B—C1B	177.34 (15)	C7A—C1A—N3A—C4A	−179.07 (16)
C1B—C2B—C3B—C4B	−176.64 (17)	C1A—N3A—C4A—N4A	177.07 (16)
S1—C2B—C3B—C4B	0.32 (19)	C1A—N3A—C4A—C5A	−2.6 (2)

C1B—C2B—C3B—Br1	2.0 (3)	N4A—C4A—C5A—C6A	−176.19 (17)
S1—C2B—C3B—Br1	178.93 (9)	N3A—C4A—C5A—C6A	3.4 (3)
Br1^{i}—Br1—C3B—C2B	−39.37 (17)	N4A—C4A—C5A—Cl1	4.3 (2)
Cl1^{ii}—Br1—C3B—C2B	−162.85 (14)	N3A—C4A—C5A—Cl1	−176.06 (13)
S1^{iii}—Br1—C3B—C2B	−94.57 (15)	C1A—N1A—C6A—C5A	−0.6 (3)
Br1^{i}—Br1—C3B—C4B	139.14 (12)	C1A—N1A—C6A—C8A	−179.97 (16)
Cl1^{ii}—Br1—C3B—C4B	15.66 (15)	C4A—C5A—C6A—N1A	−1.8 (3)
S1^{iii}—Br1—C3B—C4B	83.94 (14)	Cl1—C5A—C6A—N1A	177.67 (13)
C2B—C3B—C4B—C5B	−0.6 (2)	C4A—C5A—C6A—C8A	177.52 (17)
Br1—C3B—C4B—C5B	−179.30 (13)	Cl1—C5A—C6A—C8A	−3.0 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*B*—H1*A*···N1*A*	0.89 (3)	1.73 (4)	2.618 (2)	172 (3)
C5*B*—H5*AA*···Br1^{iv}	0.95	2.92	3.6281 (18)	133
N4*A*—H4*B*1···N3*A*^{v}	0.81 (3)	2.25 (3)	3.058 (2)	176 (3)
N4*A*—H4*B*2···O2*B*^{vi}	0.83 (3)	2.23 (3)	2.965 (2)	148 (3)
C8*A*—H8*B*4···Cl1	0.98	2.59	3.119 (2)	114

Symmetry codes: (iv) *x*+1, *y*, *z*; (v) −*x*, −*y*+2, −*z*+1; (vi) −*x*, −*y*+1, −*z*+1.

4-Amino-5-chloro-2,6-dimethylpyrimidine–5-chlorothiophene-2-carboxylic acid (1/1) (COCRYSTAL-2)

Crystal data

$C_6H_8ClN_3·C_5H_3ClO_2S$
M_r = 320.19
Triclinic, $P\overline{1}$
a = 7.2182 (3) Å
b = 7.6364 (3) Å
c = 12.7516 (6) Å
α = 90.707 (2)°
β = 102.629 (2)°
γ = 105.338 (2)°
V = 659.61 (5) Å^3
Z = 2
F(000) = 328
D_x = 1.612 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5911 reflections
θ = 2.8–29.6°
μ = 0.65 mm^{-1}
T = 100 K
Rod, colourless
0.37 × 0.19 × 0.11 mm

Data collection

Bruker D8 Quest CMOS diffractometer
Radiation source: I-mu-S microsource X-ray tube
ω and phi scans
Absorption correction: multi-scan (APEX2; Bruker, 2014)
T_{min} = 0.477, T_{max} = 0.746
8796 measured reflections
3636 independent reflections
2947 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 29.6°, θ_{min} = 2.8°
h = −10→9
k = −10→10
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.138
S = 1.15
3636 reflections
187 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 0.5883P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.76$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1B	−0.28477 (8)	−0.34293 (8)	0.00245 (5)	0.01882 (16)	
S1B	0.04024 (8)	−0.07368 (8)	0.15616 (5)	0.01421 (15)	
O1B	0.3910 (3)	0.1819 (2)	0.29123 (14)	0.0189 (4)	
H1A	0.498 (6)	0.281 (6)	0.332 (4)	0.059 (13)*	
O2B	0.6159 (2)	0.1262 (3)	0.20660 (15)	0.0212 (4)	
C1B	0.4469 (3)	0.0974 (3)	0.21763 (19)	0.0155 (5)	
C2B	0.2832 (3)	−0.0399 (3)	0.14660 (18)	0.0133 (4)	
C3B	0.2971 (3)	−0.1483 (3)	0.06501 (19)	0.0153 (4)	
H3AA	0.418792	−0.147819	0.047805	0.018*	
C4B	0.1128 (3)	−0.2620 (3)	0.00817 (19)	0.0161 (5)	
H4AA	0.096144	−0.346000	−0.050993	0.019*	
C5B	−0.0382 (3)	−0.2356 (3)	0.04925 (18)	0.0142 (4)	
Cl1A	0.94838 (8)	0.51403 (8)	0.72886 (4)	0.01724 (15)	
N1A	0.6580 (3)	0.4397 (3)	0.42204 (16)	0.0134 (4)	
C2A	0.7088 (3)	0.6114 (3)	0.39334 (18)	0.0128 (4)	
N3A	0.8311 (3)	0.7539 (3)	0.45660 (15)	0.0133 (4)	
N4A	1.0414 (3)	0.8636 (3)	0.62157 (16)	0.0144 (4)	
H4B1	1.076 (5)	0.974 (5)	0.602 (3)	0.035 (9)*	
H4B2	1.119 (4)	0.855 (4)	0.683 (3)	0.021 (8)*	
C4A	0.9120 (3)	0.7244 (3)	0.55926 (18)	0.0117 (4)	
C5A	0.8567 (3)	0.5476 (3)	0.59597 (17)	0.0119 (4)	
C6A	0.7326 (3)	0.4068 (3)	0.52538 (18)	0.0135 (4)	
C7A	0.6204 (4)	0.6424 (4)	0.27936 (19)	0.0177 (5)	
H7BA	0.652565	0.773352	0.270051	0.027*	
H7BB	0.476747	0.591891	0.264024	0.027*	
H7BC	0.674362	0.582116	0.229662	0.027*	
C8A	0.6708 (4)	0.2145 (3)	0.5550 (2)	0.0171 (5)	
H8B1	0.610279	0.133235	0.489367	0.026*	0.50 (4)
H8B2	0.574907	0.204034	0.600045	0.026*	0.50 (4)
H8B3	0.786587	0.180211	0.595054	0.026*	0.50 (4)
H8B4	0.718728	0.209791	0.632726	0.026*	0.50 (4)
H8B5	0.726639	0.137893	0.515809	0.026*	0.50 (4)

H8B6	0.526406	0.169796	0.535931	0.026*	0.50 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1B	0.0139 (3)	0.0185 (3)	0.0179 (3)	−0.0015 (2)	−0.0017 (2)	−0.0007 (2)
S1B	0.0142 (3)	0.0142 (3)	0.0121 (3)	0.0010 (2)	0.0022 (2)	−0.0021 (2)
O1B	0.0167 (8)	0.0180 (9)	0.0170 (9)	−0.0026 (7)	0.0025 (7)	−0.0078 (7)
O2B	0.0129 (8)	0.0256 (10)	0.0209 (9)	0.0020 (7)	−0.0009 (7)	−0.0037 (7)
C1B	0.0169 (11)	0.0118 (11)	0.0139 (11)	0.0007 (9)	−0.0007 (8)	0.0001 (9)
C2B	0.0114 (10)	0.0147 (11)	0.0116 (10)	0.0018 (8)	−0.0002 (8)	0.0022 (8)
C3B	0.0141 (10)	0.0150 (11)	0.0158 (11)	0.0036 (9)	0.0022 (8)	0.0009 (9)
C4B	0.0195 (11)	0.0152 (11)	0.0099 (10)	0.0023 (9)	−0.0013 (8)	−0.0041 (9)
C5B	0.0143 (10)	0.0127 (11)	0.0118 (10)	0.0007 (8)	−0.0015 (8)	0.0001 (8)
Cl1A	0.0200 (3)	0.0183 (3)	0.0099 (3)	0.0019 (2)	0.0002 (2)	0.0015 (2)
N1A	0.0117 (9)	0.0128 (9)	0.0131 (9)	−0.0008 (7)	0.0028 (7)	−0.0024 (7)
C2A	0.0107 (10)	0.0156 (11)	0.0106 (10)	0.0022 (8)	0.0014 (8)	−0.0028 (8)
N3A	0.0122 (9)	0.0143 (9)	0.0120 (9)	0.0018 (7)	0.0022 (7)	0.0001 (7)
N4A	0.0167 (9)	0.0121 (10)	0.0101 (9)	−0.0005 (8)	−0.0002 (7)	−0.0025 (8)
C4A	0.0105 (10)	0.0125 (10)	0.0120 (10)	0.0036 (8)	0.0018 (8)	−0.0009 (8)
C5A	0.0127 (10)	0.0145 (11)	0.0071 (9)	0.0025 (8)	0.0010 (7)	−0.0001 (8)
C6A	0.0142 (10)	0.0142 (11)	0.0122 (10)	0.0026 (9)	0.0046 (8)	−0.0008 (8)
C7A	0.0178 (11)	0.0220 (12)	0.0118 (11)	0.0045 (10)	0.0013 (8)	0.0029 (9)
C8A	0.0193 (11)	0.0103 (11)	0.0171 (11)	−0.0026 (9)	0.0031 (9)	0.0006 (9)

Geometric parameters (Å, º)

Cl1B—C5B	1.717 (2)	N3A—C4A	1.360 (3)
S1B—C5B	1.720 (2)	N4A—C4A	1.328 (3)
S1B—C2B	1.735 (2)	N4A—H4B1	0.87 (4)
O1B—C1B	1.322 (3)	N4A—H4B2	0.87 (3)
O1B—H1A	0.97 (5)	C4A—C5A	1.419 (3)
O2B—C1B	1.221 (3)	C5A—C6A	1.372 (3)
C1B—C2B	1.473 (3)	C6A—C8A	1.497 (3)
C2B—C3B	1.359 (3)	C7A—H7BA	0.9800
C3B—C4B	1.414 (3)	C7A—H7BB	0.9800
C3B—H3AA	0.9500	C7A—H7BC	0.9800
C4B—C5B	1.366 (3)	C8A—H8B1	0.9800
C4B—H4AA	0.9500	C8A—H8B2	0.9800
Cl1A—C5A	1.728 (2)	C8A—H8B3	0.9800
N1A—C2A	1.343 (3)	C8A—H8B4	0.9800
N1A—C6A	1.364 (3)	C8A—H8B5	0.9800
C2A—N3A	1.332 (3)	C8A—H8B6	0.9800
C2A—C7A	1.503 (3)		
C5B—S1B—C2B	90.45 (11)	N4A—C4A—C5A	122.4 (2)
C1B—O1B—H1A	113 (3)	N3A—C4A—C5A	119.4 (2)
O2B—C1B—O1B	125.2 (2)	C6A—C5A—C4A	119.5 (2)

O2B—C1B—C2B	121.2 (2)	C6A—C5A—Cl1A	121.36 (18)
O1B—C1B—C2B	113.6 (2)	C4A—C5A—Cl1A	119.13 (17)
C3B—C2B—C1B	126.5 (2)	N1A—C6A—C5A	119.7 (2)
C3B—C2B—S1B	111.65 (18)	N1A—C6A—C8A	116.7 (2)
C1B—C2B—S1B	121.84 (18)	C5A—C6A—C8A	123.7 (2)
C2B—C3B—C4B	113.5 (2)	C2A—C7A—H7BA	109.5
C2B—C3B—H3AA	123.3	C2A—C7A—H7BB	109.5
C4B—C3B—H3AA	123.3	H7BA—C7A—H7BB	109.5
C5B—C4B—C3B	111.3 (2)	C2A—C7A—H7BC	109.5
C5B—C4B—H4AA	124.3	H7BA—C7A—H7BC	109.5
C3B—C4B—H4AA	124.3	H7BB—C7A—H7BC	109.5
C4B—C5B—Cl1B	126.31 (19)	C6A—C8A—H8B1	109.5
C4B—C5B—S1B	113.09 (18)	C6A—C8A—H8B2	109.5
Cl1B—C5B—S1B	120.59 (14)	H8B1—C8A—H8B2	109.5
C2A—N1A—C6A	118.1 (2)	C6A—C8A—H8B3	109.5
N3A—C2A—N1A	125.6 (2)	H8B1—C8A—H8B3	109.5
N3A—C2A—C7A	118.0 (2)	H8B2—C8A—H8B3	109.5
N1A—C2A—C7A	116.4 (2)	C6A—C8A—H8B4	109.5
C2A—N3A—C4A	117.65 (19)	C6A—C8A—H8B5	109.5
C4A—N4A—H4B1	124 (2)	H8B4—C8A—H8B5	109.5
C4A—N4A—H4B2	125 (2)	C6A—C8A—H8B6	109.5
H4B1—N4A—H4B2	110 (3)	H8B4—C8A—H8B6	109.5
N4A—C4A—N3A	118.2 (2)	H8B5—C8A—H8B6	109.5

O2B—C1B—C2B—C3B	0.8 (4)	N1A—C2A—N3A—C4A	−0.1 (3)
O1B—C1B—C2B—C3B	−179.3 (2)	C7A—C2A—N3A—C4A	−179.31 (19)
O2B—C1B—C2B—S1B	−176.30 (18)	C2A—N3A—C4A—N4A	176.8 (2)
O1B—C1B—C2B—S1B	3.6 (3)	C2A—N3A—C4A—C5A	−2.9 (3)
C5B—S1B—C2B—C3B	0.25 (18)	N4A—C4A—C5A—C6A	−175.5 (2)
C5B—S1B—C2B—C1B	177.78 (19)	N3A—C4A—C5A—C6A	4.3 (3)
C1B—C2B—C3B—C4B	−177.6 (2)	N4A—C4A—C5A—Cl1A	4.2 (3)
S1B—C2B—C3B—C4B	−0.2 (3)	N3A—C4A—C5A—Cl1A	−176.07 (16)
C2B—C3B—C4B—C5B	0.0 (3)	C2A—N1A—C6A—C5A	−0.4 (3)
C3B—C4B—C5B—Cl1B	178.81 (17)	C2A—N1A—C6A—C8A	179.17 (19)
C3B—C4B—C5B—S1B	0.1 (3)	C4A—C5A—C6A—N1A	−2.5 (3)
C2B—S1B—C5B—C4B	−0.22 (19)	Cl1A—C5A—C6A—N1A	177.80 (16)
C2B—S1B—C5B—Cl1B	−178.97 (15)	C4A—C5A—C6A—C8A	177.9 (2)
C6A—N1A—C2A—N3A	1.8 (3)	Cl1A—C5A—C6A—C8A	−1.7 (3)
C6A—N1A—C2A—C7A	−178.94 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*B*—H1*A*···N1*A*	0.97 (5)	1.66 (5)	2.623 (3)	169 (4)
C4*B*—H4*AA*···Cl1*A*^{i}	0.95	2.86	3.734 (2)	154
N4*A*—H4*B*1···N3*A*^{ii}	0.87 (4)	2.20 (4)	3.070 (3)	176 (3)
N4*A*—H4*B*2···O2*B*^{iii}	0.87 (3)	2.08 (3)	2.907 (3)	157 (3)
C7*A*—H7*BB*···Cl1*A*^{iv}	0.98	2.98	3.938 (2)	166

C7*A*—H7*BC*···Cl1*A*^{iii}	0.98	2.94	3.638 (2)	129
C8*A*—H8*B*4···Cl1*A*	0.98	2.58	3.110 (3)	114
C8*A*—H8*B*5···N4*A*^{iii}	0.98	2.68	3.523 (3)	145

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

4-Amino-5-chloro-2,6-dimethylpyrimidine—2,4-dichlorobenzoic acid (1/1) (COCRYSTAL-3)

Crystal data

$C_6H_8ClN_3·C_7H_4Cl_2O_2$
M_r = 348.61
Triclinic, $P\overline{1}$
a = 7.3015 (4) Å
b = 7.5060 (6) Å
c = 14.9665 (8) Å
α = 92.539 (5)°
β = 98.522 (5)°
γ = 113.657 (7)°
V = 738.12 (9) Å^3
Z = 2
F(000) = 356
D_x = 1.568 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 2184 reflections
θ = 3.0–75.8°
μ = 5.70 mm^{-1}
T = 120 K
Plate, colorless
0.51 × 0.35 × 0.08 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: sealed X-ray tube
Detector resolution: 10.6501 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.538, T_{max} = 1.000
5965 measured reflections
3050 independent reflections
2546 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 76.9°, θ_{min} = 3.0°
h = −4→9
k = −9→8
l = −18→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.135
S = 1.05
3050 reflections
204 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0781P)^2 + 0.423P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.92360 (9)	0.67568 (9)	1.08079 (4)	0.02879 (18)
N1A	0.5642 (3)	0.4615 (3)	0.84009 (15)	0.0255 (5)
C2A	0.4796 (4)	0.2733 (4)	0.85176 (17)	0.0249 (5)
N3A	0.5203 (3)	0.1957 (3)	0.92717 (15)	0.0239 (4)

N4A	0.6923 (4)	0.2415 (4)	1.07384 (16)	0.0278 (5)
H41	0.624 (5)	0.118 (5)	1.077 (2)	0.024 (8)*
H42	0.760 (6)	0.318 (6)	1.124 (3)	0.047 (11)*
C4A	0.6537 (4)	0.3192 (4)	0.99820 (17)	0.0232 (5)
C5A	0.7488 (4)	0.5206 (4)	0.98982 (18)	0.0246 (5)
C6A	0.7034 (4)	0.5891 (4)	0.90944 (18)	0.0251 (5)
C7A	0.3234 (4)	0.1328 (4)	0.77562 (18)	0.0295 (6)
H7AA	0.2789	0.2062	0.7313	0.044*
H7AB	0.2064	0.0450	0.8001	0.044*
H7AC	0.3828	0.0556	0.7458	0.044*
C8A	0.8001 (5)	0.7990 (4)	0.8943 (2)	0.0349 (6)
H8AA	0.7555	0.8135	0.8310	0.052*
H8AB	0.9483	0.8446	0.9068	0.052*
H8AC	0.7600	0.8771	0.9351	0.052*
Cl2	−0.04948 (10)	0.74463 (11)	0.61458 (4)	0.03186 (19)
Cl3	0.20778 (12)	0.87604 (12)	0.29833 (4)	0.0372 (2)
O1B	0.4692 (4)	0.5681 (4)	0.68251 (15)	0.0382 (5)
H1B	0.503 (7)	0.540 (8)	0.739 (4)	0.080 (16)*
O2B	0.2353 (4)	0.6429 (4)	0.73334 (14)	0.0446 (6)
C1B	0.2906 (4)	0.6968 (4)	0.58101 (17)	0.0243 (5)
C2B	0.1298 (4)	0.7480 (4)	0.54990 (18)	0.0253 (5)
C3B	0.1030 (4)	0.8021 (4)	0.46282 (18)	0.0275 (5)
H3BA	−0.0074	0.8352	0.4420	0.033*
C4B	0.2400 (4)	0.8069 (4)	0.40696 (17)	0.0269 (5)
C5B	0.4022 (4)	0.7595 (4)	0.43580 (19)	0.0297 (6)
H5BA	0.4956	0.7643	0.3970	0.036*
C6B	0.4252 (4)	0.7051 (4)	0.52212 (19)	0.0280 (6)
H6BA	0.5361	0.6721	0.5423	0.034*
C7B	0.3271 (4)	0.6335 (4)	0.67360 (18)	0.0262 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0287 (3)	0.0286 (3)	0.0280 (3)	0.0116 (3)	0.0029 (2)	0.0030 (2)
N1A	0.0263 (11)	0.0300 (11)	0.0245 (10)	0.0148 (9)	0.0056 (9)	0.0107 (9)
C2A	0.0243 (12)	0.0306 (13)	0.0246 (12)	0.0154 (10)	0.0056 (10)	0.0079 (10)
N3A	0.0246 (10)	0.0270 (11)	0.0236 (10)	0.0131 (9)	0.0054 (8)	0.0093 (8)
N4A	0.0312 (12)	0.0272 (12)	0.0237 (11)	0.0110 (10)	0.0021 (9)	0.0100 (9)
C4A	0.0220 (11)	0.0282 (13)	0.0240 (12)	0.0137 (10)	0.0064 (9)	0.0075 (10)
C5A	0.0250 (12)	0.0271 (13)	0.0245 (12)	0.0131 (10)	0.0053 (10)	0.0056 (10)
C6A	0.0239 (12)	0.0281 (13)	0.0291 (13)	0.0150 (10)	0.0077 (10)	0.0098 (10)
C7A	0.0320 (13)	0.0322 (14)	0.0245 (12)	0.0140 (11)	0.0029 (11)	0.0076 (10)
C8A	0.0362 (15)	0.0311 (15)	0.0389 (16)	0.0147 (12)	0.0059 (12)	0.0141 (12)
Cl2	0.0287 (3)	0.0419 (4)	0.0303 (3)	0.0192 (3)	0.0063 (3)	0.0086 (3)
Cl3	0.0436 (4)	0.0511 (4)	0.0232 (3)	0.0265 (3)	0.0023 (3)	0.0115 (3)
O1B	0.0455 (12)	0.0577 (14)	0.0298 (11)	0.0366 (11)	0.0114 (9)	0.0233 (10)
O2B	0.0569 (14)	0.0731 (17)	0.0245 (10)	0.0463 (13)	0.0097 (10)	0.0133 (10)
C1B	0.0267 (12)	0.0211 (12)	0.0228 (12)	0.0092 (10)	−0.0004 (9)	0.0021 (9)

C2B	0.0262 (12)	0.0239 (12)	0.0258 (12)	0.0109 (10)	0.0030 (10)	0.0042 (9)
C3B	0.0274 (12)	0.0268 (13)	0.0269 (13)	0.0123 (11)	−0.0025 (10)	0.0034 (10)
C4B	0.0342 (14)	0.0271 (13)	0.0190 (11)	0.0133 (11)	0.0007 (10)	0.0053 (9)
C5B	0.0317 (14)	0.0338 (14)	0.0263 (13)	0.0163 (12)	0.0048 (11)	0.0062 (11)
C6B	0.0290 (13)	0.0320 (14)	0.0270 (13)	0.0176 (11)	0.0016 (10)	0.0066 (10)
C7B	0.0301 (13)	0.0243 (12)	0.0250 (12)	0.0127 (11)	0.0026 (10)	0.0037 (10)

Geometric parameters (Å, º)

Cl1—C5A	1.729 (3)	C8A—H8AC	0.9800
N1A—C2A	1.327 (4)	Cl2—C2B	1.733 (3)
N1A—C6A	1.359 (4)	Cl3—C4B	1.740 (3)
C2A—N3A	1.341 (3)	O1B—C7B	1.307 (3)
C2A—C7A	1.502 (4)	O1B—H1B	0.90 (5)
N3A—C4A	1.349 (3)	O2B—C7B	1.210 (4)
N4A—C4A	1.340 (3)	C1B—C6B	1.399 (4)
N4A—H41	0.87 (4)	C1B—C2B	1.400 (4)
N4A—H42	0.87 (4)	C1B—C7B	1.506 (3)
C4A—C5A	1.408 (4)	C2B—C3B	1.392 (4)
C5A—C6A	1.377 (4)	C3B—C4B	1.387 (4)
C6A—C8A	1.489 (4)	C3B—H3BA	0.9500
C7A—H7AA	0.9800	C4B—C5B	1.384 (4)
C7A—H7AB	0.9800	C5B—C6B	1.379 (4)
C7A—H7AC	0.9800	C5B—H5BA	0.9500
C8A—H8AA	0.9800	C6B—H6BA	0.9500
C8A—H8AB	0.9800		

C2A—N1A—C6A	118.5 (2)	C6A—C8A—H8AC	109.5
N1A—C2A—N3A	125.4 (2)	H8AA—C8A—H8AC	109.5
N1A—C2A—C7A	118.4 (2)	H8AB—C8A—H8AC	109.5
N3A—C2A—C7A	116.2 (2)	C7B—O1B—H1B	115 (3)
C2A—N3A—C4A	117.6 (2)	C6B—C1B—C2B	117.7 (2)
C4A—N4A—H41	119 (2)	C6B—C1B—C7B	118.3 (2)
C4A—N4A—H42	119 (3)	C2B—C1B—C7B	124.0 (2)
H41—N4A—H42	119 (3)	C3B—C2B—C1B	121.0 (2)
N4A—C4A—N3A	117.5 (2)	C3B—C2B—Cl2	115.8 (2)
N4A—C4A—C5A	122.9 (2)	C1B—C2B—Cl2	123.2 (2)
N3A—C4A—C5A	119.6 (2)	C4B—C3B—C2B	118.9 (2)
C6A—C5A—C4A	119.6 (2)	C4B—C3B—H3BA	120.5
C6A—C5A—Cl1	121.5 (2)	C2B—C3B—H3BA	120.5
C4A—C5A—Cl1	118.9 (2)	C5B—C4B—C3B	121.6 (2)
N1A—C6A—C5A	119.3 (2)	C5B—C4B—Cl3	119.4 (2)
N1A—C6A—C8A	117.7 (2)	C3B—C4B—Cl3	119.0 (2)
C5A—C6A—C8A	123.0 (3)	C6B—C5B—C4B	118.5 (3)
C2A—C7A—H7AA	109.5	C6B—C5B—H5BA	120.8
C2A—C7A—H7AB	109.5	C4B—C5B—H5BA	120.8
H7AA—C7A—H7AB	109.5	C5B—C6B—C1B	122.2 (3)
C2A—C7A—H7AC	109.5	C5B—C6B—H6BA	118.9

H7AA—C7A—H7AC	109.5	C1B—C6B—H6BA	118.9
H7AB—C7A—H7AC	109.5	O2B—C7B—O1B	123.7 (2)
C6A—C8A—H8AA	109.5	O2B—C7B—C1B	123.7 (2)
C6A—C8A—H8AB	109.5	O1B—C7B—C1B	112.7 (2)
H8AA—C8A—H8AB	109.5		

C6A—N1A—C2A—N3A	−0.2 (4)	C7B—C1B—C2B—C3B	−178.9 (2)
C6A—N1A—C2A—C7A	179.1 (2)	C6B—C1B—C2B—Cl2	179.8 (2)
N1A—C2A—N3A—C4A	2.0 (4)	C7B—C1B—C2B—Cl2	−0.1 (4)
C7A—C2A—N3A—C4A	−177.3 (2)	C1B—C2B—C3B—C4B	−0.7 (4)
C2A—N3A—C4A—N4A	179.3 (2)	Cl2—C2B—C3B—C4B	−179.6 (2)
C2A—N3A—C4A—C5A	−2.0 (4)	C2B—C3B—C4B—C5B	−0.1 (4)
N4A—C4A—C5A—C6A	179.1 (2)	C2B—C3B—C4B—Cl3	−179.6 (2)
N3A—C4A—C5A—C6A	0.4 (4)	C3B—C4B—C5B—C6B	0.5 (4)
N4A—C4A—C5A—Cl1	0.1 (4)	Cl3—C4B—C5B—C6B	180.0 (2)
N3A—C4A—C5A—Cl1	−178.59 (19)	C4B—C5B—C6B—C1B	−0.1 (4)
C2A—N1A—C6A—C5A	−1.5 (4)	C2B—C1B—C6B—C5B	−0.6 (4)
C2A—N1A—C6A—C8A	178.6 (2)	C7B—C1B—C6B—C5B	179.3 (3)
C4A—C5A—C6A—N1A	1.4 (4)	C6B—C1B—C7B—O2B	171.1 (3)
Cl1—C5A—C6A—N1A	−179.66 (19)	C2B—C1B—C7B—O2B	−8.9 (4)
C4A—C5A—C6A—C8A	−178.8 (2)	C6B—C1B—C7B—O1B	−8.7 (4)
Cl1—C5A—C6A—C8A	0.2 (4)	C2B—C1B—C7B—O1B	171.3 (3)
C6B—C1B—C2B—C3B	1.1 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4*A*—H41···N3*A*^{i}	0.87 (4)	2.15 (4)	3.014 (3)	172 (3)
N4*A*—H42···O2*B*^{ii}	0.87 (4)	2.14 (4)	2.884 (3)	143 (4)
O1*B*—H1*B*···N1*A*	0.90 (5)	1.71 (5)	2.610 (3)	174 (5)

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

4-Amino-5-chloro-2,6-dimethylpyrimidine–2-aminobenzoic acid (1/1) (COCRYSTAL-4)

Crystal data

$C_6H_8ClN_3·C_7H_7NO_2$
M_r = 294.74
Monoclinic, $P2_1/n$
a = 8.0965 (2) Å
b = 7.2427 (3) Å
c = 24.0738 (9) Å
β = 90.831 (3)°
V = 1411.55 (9) Å^3
Z = 4
F(000) = 616
D_x = 1.387 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3296 reflections
θ = 3.7–76.5°
μ = 2.47 mm^{-1}
T = 120 K
The symmetry employed for this shelxl refinement is uniquely defined by the following loop, which should always be used as a source of symmetry information in preference to the above space-group names. They are only intended as comments., pale yellow-orange
0.46 × 0.22 × 0.06 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: sealed X-ray tube
Detector resolution: 10.6501 pixels mm^{-1}
ω scans
Absorption correction: analytical [CrysAlis PRO (Oxford Diffraction, 2011), based on expressions derived by Clark & Reid (1995)]
T_{min} = 0.547, T_{max} = 0.877
6899 measured reflections
2927 independent reflections
2481 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 76.7°, θ_{min} = 3.7°
h = −10→6
k = −8→9
l = −30→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.110
S = 1.05
2927 reflections
203 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 0.465P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.11199 (5)	0.49692 (6)	0.38012 (2)	0.02408 (14)
N1A	0.27995 (17)	0.51697 (19)	0.53553 (6)	0.0192 (3)
C2A	0.22132 (19)	0.6818 (2)	0.55060 (7)	0.0198 (3)
N3A	0.12834 (16)	0.79300 (19)	0.51880 (6)	0.0189 (3)
N4A	−0.00933 (18)	0.8419 (2)	0.43543 (6)	0.0213 (3)
H4A1	−0.048 (3)	0.946 (4)	0.4501 (10)	0.034 (6)*
H4A2	−0.050 (3)	0.800 (4)	0.4043 (11)	0.042 (7)*
C4A	0.08865 (19)	0.7343 (2)	0.46684 (7)	0.0179 (3)
C5A	0.15295 (19)	0.5643 (2)	0.44778 (7)	0.0187 (3)
C6A	0.24751 (19)	0.4579 (2)	0.48289 (7)	0.0194 (3)
C7A	0.2642 (2)	0.7482 (3)	0.60803 (7)	0.0259 (4)
H7AA	0.1778	0.8320	0.6209	0.039*
H7AB	0.3701	0.8137	0.6075	0.039*
H7AC	0.2728	0.6423	0.6333	0.039*
C8A	0.3162 (2)	0.2746 (3)	0.46605 (7)	0.0246 (4)
H8AA	0.3960	0.2322	0.4943	0.037*
H8AB	0.3715	0.2869	0.4303	0.037*
H8AC	0.2262	0.1847	0.4625	0.037*
O1B	0.46209 (15)	0.30141 (19)	0.59902 (5)	0.0268 (3)
H1B	0.379 (4)	0.383 (5)	0.5759 (14)	0.083 (11)*
O2B	0.25284 (14)	0.25583 (18)	0.65694 (5)	0.0242 (3)

N1B	0.2989 (2)	0.0084 (2)	0.74083 (7)	0.0299 (4)
H1B1	0.225 (3)	0.086 (4)	0.7235 (10)	0.038 (6)*
H1B2	0.275 (3)	−0.052 (4)	0.7695 (11)	0.042 (7)*
C1B	0.50618 (19)	0.0925 (2)	0.67226 (7)	0.0188 (3)
C2B	0.4524 (2)	−0.0091 (2)	0.71897 (7)	0.0200 (3)
C3B	0.5643 (2)	−0.1364 (2)	0.74338 (7)	0.0244 (4)
H3BA	0.5304	−0.2075	0.7744	0.029*
C4B	0.7206 (2)	−0.1595 (3)	0.72327 (8)	0.0265 (4)
H4BA	0.7931	−0.2459	0.7406	0.032*
C5B	0.7748 (2)	−0.0575 (3)	0.67756 (8)	0.0250 (4)
H5BA	0.8837	−0.0726	0.6641	0.030*
C6B	0.6672 (2)	0.0649 (2)	0.65261 (7)	0.0208 (3)
H6BA	0.7026	0.1329	0.6212	0.025*
C7B	0.3958 (2)	0.2228 (2)	0.64266 (7)	0.0197 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0307 (2)	0.0245 (2)	0.0170 (2)	0.00267 (15)	−0.00203 (16)	−0.00299 (15)
N1A	0.0199 (6)	0.0193 (7)	0.0182 (7)	0.0009 (5)	−0.0010 (5)	0.0013 (5)
C2A	0.0193 (7)	0.0194 (8)	0.0207 (8)	−0.0019 (6)	−0.0001 (6)	0.0002 (6)
N3A	0.0204 (6)	0.0183 (7)	0.0180 (7)	0.0001 (5)	−0.0005 (5)	0.0011 (5)
N4A	0.0240 (7)	0.0209 (7)	0.0189 (7)	0.0035 (6)	−0.0033 (6)	0.0008 (6)
C4A	0.0179 (7)	0.0177 (8)	0.0182 (7)	−0.0020 (6)	0.0013 (6)	0.0017 (6)
C5A	0.0210 (7)	0.0185 (8)	0.0165 (7)	−0.0010 (6)	0.0010 (6)	−0.0003 (6)
C6A	0.0189 (7)	0.0196 (8)	0.0197 (8)	−0.0011 (6)	0.0021 (6)	0.0005 (6)
C7A	0.0307 (9)	0.0244 (9)	0.0225 (8)	0.0027 (7)	−0.0060 (7)	−0.0031 (7)
C8A	0.0263 (8)	0.0227 (9)	0.0248 (8)	0.0045 (7)	0.0006 (7)	−0.0014 (7)
O1B	0.0246 (6)	0.0320 (7)	0.0239 (6)	0.0051 (5)	0.0017 (5)	0.0103 (5)
O2B	0.0229 (6)	0.0283 (7)	0.0213 (6)	0.0043 (5)	0.0006 (5)	0.0003 (5)
N1B	0.0282 (8)	0.0341 (9)	0.0275 (8)	0.0037 (7)	0.0068 (7)	0.0111 (7)
C1B	0.0214 (7)	0.0181 (8)	0.0170 (7)	−0.0003 (6)	−0.0025 (6)	−0.0017 (6)
C2B	0.0231 (8)	0.0195 (8)	0.0175 (8)	−0.0015 (6)	−0.0024 (6)	−0.0015 (6)
C3B	0.0324 (9)	0.0213 (9)	0.0194 (8)	−0.0008 (7)	−0.0027 (7)	0.0021 (7)
C4B	0.0318 (9)	0.0222 (9)	0.0252 (9)	0.0050 (7)	−0.0077 (7)	0.0016 (7)
C5B	0.0232 (8)	0.0263 (9)	0.0256 (9)	0.0053 (7)	−0.0010 (7)	−0.0006 (7)
C6B	0.0234 (8)	0.0202 (8)	0.0186 (8)	−0.0009 (6)	−0.0001 (6)	−0.0008 (7)
C7B	0.0218 (7)	0.0209 (8)	0.0164 (7)	−0.0010 (6)	−0.0020 (6)	−0.0014 (6)

Geometric parameters (Å, º)

Cl1—C5A	1.7279 (16)	O1B—C7B	1.316 (2)
N1A—C2A	1.337 (2)	O1B—H1B	1.05 (4)
N1A—C6A	1.360 (2)	O2B—C7B	1.235 (2)
C2A—N3A	1.336 (2)	N1B—C2B	1.363 (2)
C2A—C7A	1.500 (2)	N1B—H1B1	0.91 (3)
N3A—C4A	1.355 (2)	N1B—H1B2	0.84 (3)
N4A—C4A	1.338 (2)	C1B—C6B	1.408 (2)

N4A—H4A1	0.89 (3)	C1B—C2B	1.417 (2)
N4A—H4A2	0.87 (3)	C1B—C7B	1.476 (2)
C4A—C5A	1.416 (2)	C2B—C3B	1.415 (2)
C5A—C6A	1.369 (2)	C3B—C4B	1.372 (3)
C6A—C8A	1.497 (2)	C3B—H3BA	0.9500
C7A—H7AA	0.9800	C4B—C5B	1.401 (3)
C7A—H7AB	0.9800	C4B—H4BA	0.9500
C7A—H7AC	0.9800	C5B—C6B	1.375 (2)
C8A—H8AA	0.9800	C5B—H5BA	0.9500
C8A—H8AB	0.9800	C6B—H6BA	0.9500
C8A—H8AC	0.9800		

C2A—N1A—C6A	118.00 (15)	H8AA—C8A—H8AC	109.5
N3A—C2A—N1A	125.62 (16)	H8AB—C8A—H8AC	109.5
N3A—C2A—C7A	117.11 (15)	C7B—O1B—H1B	113.6 (18)
N1A—C2A—C7A	117.28 (15)	C2B—N1B—H1B1	118.2 (15)
C2A—N3A—C4A	117.63 (15)	C2B—N1B—H1B2	119.2 (18)
C4A—N4A—H4A1	118.4 (16)	H1B1—N1B—H1B2	123 (2)
C4A—N4A—H4A2	119.7 (17)	C6B—C1B—C2B	119.32 (15)
H4A1—N4A—H4A2	121 (2)	C6B—C1B—C7B	119.05 (15)
N4A—C4A—N3A	118.01 (15)	C2B—C1B—C7B	121.61 (14)
N4A—C4A—C5A	122.76 (15)	N1B—C2B—C3B	118.84 (16)
N3A—C4A—C5A	119.23 (15)	N1B—C2B—C1B	123.39 (16)
C6A—C5A—C4A	119.62 (15)	C3B—C2B—C1B	117.77 (15)
C6A—C5A—Cl1	121.40 (13)	C4B—C3B—C2B	121.41 (16)
C4A—C5A—Cl1	118.98 (13)	C4B—C3B—H3BA	119.3
N1A—C6A—C5A	119.79 (16)	C2B—C3B—H3BA	119.3
N1A—C6A—C8A	117.64 (15)	C3B—C4B—C5B	120.93 (17)
C5A—C6A—C8A	122.56 (15)	C3B—C4B—H4BA	119.5
C2A—C7A—H7AA	109.5	C5B—C4B—H4BA	119.5
C2A—C7A—H7AB	109.5	C6B—C5B—C4B	118.65 (16)
H7AA—C7A—H7AB	109.5	C6B—C5B—H5BA	120.7
C2A—C7A—H7AC	109.5	C4B—C5B—H5BA	120.7
H7AA—C7A—H7AC	109.5	C5B—C6B—C1B	121.90 (16)
H7AB—C7A—H7AC	109.5	C5B—C6B—H6BA	119.0
C6A—C8A—H8AA	109.5	C1B—C6B—H6BA	119.0
C6A—C8A—H8AB	109.5	O2B—C7B—O1B	122.20 (16)
H8AA—C8A—H8AB	109.5	O2B—C7B—C1B	123.54 (15)
C6A—C8A—H8AC	109.5	O1B—C7B—C1B	114.25 (14)

C6A—N1A—C2A—N3A	2.1 (2)	C6B—C1B—C2B—N1B	−179.98 (17)
C6A—N1A—C2A—C7A	−177.53 (14)	C7B—C1B—C2B—N1B	−1.7 (3)
N1A—C2A—N3A—C4A	0.4 (2)	C6B—C1B—C2B—C3B	−0.8 (2)
C7A—C2A—N3A—C4A	−179.93 (14)	C7B—C1B—C2B—C3B	177.48 (15)
C2A—N3A—C4A—N4A	177.65 (14)	N1B—C2B—C3B—C4B	−179.78 (17)
C2A—N3A—C4A—C5A	−3.0 (2)	C1B—C2B—C3B—C4B	1.0 (3)
N4A—C4A—C5A—C6A	−177.58 (15)	C2B—C3B—C4B—C5B	−0.1 (3)
N3A—C4A—C5A—C6A	3.1 (2)	C3B—C4B—C5B—C6B	−0.9 (3)

N4A—C4A—C5A—Cl1	3.2 (2)	C4B—C5B—C6B—C1B	1.1 (3)
N3A—C4A—C5A—Cl1	−176.17 (12)	C2B—C1B—C6B—C5B	−0.3 (3)
C2A—N1A—C6A—C5A	−2.0 (2)	C7B—C1B—C6B—C5B	−178.55 (16)
C2A—N1A—C6A—C8A	178.93 (14)	C6B—C1B—C7B—O2B	−179.88 (16)
C4A—C5A—C6A—N1A	−0.5 (2)	C2B—C1B—C7B—O2B	1.9 (3)
Cl1—C5A—C6A—N1A	178.68 (12)	C6B—C1B—C7B—O1B	0.5 (2)
C4A—C5A—C6A—C8A	178.53 (14)	C2B—C1B—C7B—O1B	−177.71 (15)
Cl1—C5A—C6A—C8A	−2.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4*A*—H4*A*1···N3*A*^{i}	0.89 (3)	2.14 (3)	3.027 (2)	176 (2)
N4*A*—H4*A*2···O2*B*^{ii}	0.87 (3)	2.23 (3)	3.034 (2)	154 (2)
C8*A*—H8*AA*···O1*B*	0.98	2.62	3.402 (2)	137
O1*B*—H1*B*···N1*A*	1.05 (4)	1.58 (4)	2.6235 (19)	170 (3)
N1*B*—H1*B*1···O2*B*	0.91 (3)	2.04 (3)	2.722 (2)	131 (2)
N1*B*—H1*B*2···O2*B*^{iii}	0.84 (3)	2.27 (3)	3.100 (2)	171 (2)

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

4-Amino-5-chloro-2,6-dimethylpyrimidine–5-methylthiophene-2-carboxylic acid (1/1) (COCRYSTAL-5)

Crystal data

$C_6H_8ClN_3·C_6H_6O_2S$
M_r = 299.77
Monoclinic, $P2_1/c$
a = 8.273 (3) Å
b = 12.746 (4) Å
c = 13.320 (4) Å
β = 102.390 (5)°
V = 1371.8 (8) Å^3
Z = 4
F(000) = 624
D_x = 1.452 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5891 reflections
θ = 2.2–31.4°
μ = 0.43 mm^{-1}
T = 100 K
Plate, colourless
0.55 × 0.50 × 0.30 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine focus sealed tube
Graphite monochromator
ω and phi scans
Absorption correction: multi-scan (APEX2; Bruker, 2014)
T_{min} = 0.608, T_{max} = 0.746
8807 measured reflections
4109 independent reflections
3735 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 31.4°, θ_{min} = 2.2°
h = −11→12
k = −17→17
l = −11→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 1.05
4109 reflections
189 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 0.5783P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.38618 (3)	0.84503 (2)	0.35758 (2)	0.01547 (8)	
N1A	0.54569 (12)	0.74068 (7)	0.64354 (7)	0.01340 (18)	
C2A	0.62308 (14)	0.65402 (8)	0.62325 (8)	0.0128 (2)	
N3A	0.63936 (12)	0.62204 (7)	0.52992 (7)	0.01266 (18)	
N4A	0.59228 (14)	0.65222 (8)	0.35501 (8)	0.0163 (2)	
H41	0.560 (2)	0.6922 (15)	0.3027 (15)	0.032 (5)*	
H42	0.647 (2)	0.5971 (15)	0.3525 (14)	0.026 (4)*	
C4A	0.57179 (13)	0.68167 (8)	0.44758 (8)	0.01177 (19)	
C5A	0.48186 (13)	0.77260 (8)	0.46351 (8)	0.01156 (19)	
C6A	0.47182 (13)	0.80027 (8)	0.56179 (8)	0.01207 (19)	
C7A	0.69907 (16)	0.58473 (10)	0.71194 (9)	0.0190 (2)	
H7A1	0.7278	0.5169	0.6859	0.028*	0.282 (19)
H7A2	0.6198	0.5740	0.7561	0.028*	0.282 (19)
H7A3	0.7992	0.6181	0.7518	0.028*	0.282 (19)
H7A4	0.7034	0.6224	0.7766	0.028*	0.718 (19)
H7A5	0.8115	0.5653	0.7064	0.028*	0.718 (19)
H7A6	0.6320	0.5212	0.7107	0.028*	0.718 (19)
C8A	0.38111 (15)	0.89640 (9)	0.58452 (9)	0.0167 (2)	
H8A1	0.3804	0.8984	0.6580	0.025*	0.717 (18)
H8A2	0.2670	0.8944	0.5444	0.025*	0.717 (18)
H8A3	0.4367	0.9591	0.5660	0.025*	0.717 (18)
H8A4	0.3424	0.9362	0.5210	0.025*	0.283 (18)
H8A5	0.4557	0.9403	0.6345	0.025*	0.283 (18)
H8A6	0.2860	0.8755	0.6129	0.025*	0.283 (18)
S1	0.94879 (4)	0.25627 (2)	0.33202 (2)	0.01614 (8)	
O1B	0.81492 (12)	0.44704 (7)	0.53060 (7)	0.02158 (19)	
H1B	0.752 (3)	0.5071 (18)	0.5248 (16)	0.044 (6)*	
O2B	0.76792 (12)	0.45470 (7)	0.35803 (7)	0.02004 (18)	
C1B	0.82798 (14)	0.41179 (9)	0.43965 (9)	0.0150 (2)	
C2B	0.92271 (14)	0.31337 (9)	0.44446 (9)	0.0145 (2)	
C3B	0.99609 (16)	0.25478 (9)	0.52815 (10)	0.0185 (2)	
H3BA	0.9950	0.2734	0.5971	0.022*	
C4B	1.07400 (16)	0.16312 (10)	0.50029 (10)	0.0200 (2)	
H4BA	1.1305	0.1137	0.5488	0.024*	
C5B	1.05905 (15)	0.15343 (9)	0.39617 (10)	0.0162 (2)	
C6B	1.12401 (17)	0.06825 (10)	0.33793 (11)	0.0232 (3)	

H6BA	1.1161	0.0007	0.3716	0.035*
H6BB	1.2400	0.0826	0.3368	0.035*
H6BC	1.0584	0.0658	0.2673	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.01899 (14)	0.01426 (13)	0.01211 (13)	0.00442 (9)	0.00102 (10)	0.00099 (8)
N1A	0.0154 (4)	0.0144 (4)	0.0109 (4)	−0.0005 (3)	0.0039 (3)	−0.0008 (3)
C2A	0.0143 (5)	0.0139 (5)	0.0105 (5)	−0.0008 (4)	0.0032 (4)	0.0004 (3)
N3A	0.0151 (4)	0.0126 (4)	0.0104 (4)	0.0015 (3)	0.0029 (3)	0.0003 (3)
N4A	0.0248 (5)	0.0146 (4)	0.0096 (4)	0.0071 (4)	0.0039 (4)	0.0000 (3)
C4A	0.0134 (5)	0.0116 (4)	0.0103 (5)	−0.0005 (4)	0.0026 (4)	−0.0011 (4)
C5A	0.0124 (5)	0.0113 (4)	0.0105 (4)	0.0007 (3)	0.0014 (4)	0.0003 (3)
C6A	0.0120 (5)	0.0120 (4)	0.0126 (5)	−0.0014 (4)	0.0034 (4)	−0.0020 (4)
C7A	0.0246 (6)	0.0203 (5)	0.0121 (5)	0.0044 (4)	0.0040 (4)	0.0040 (4)
C8A	0.0189 (5)	0.0149 (5)	0.0173 (5)	0.0025 (4)	0.0062 (4)	−0.0032 (4)
S1	0.01864 (15)	0.01600 (14)	0.01424 (14)	0.00445 (9)	0.00458 (11)	0.00057 (9)
O1B	0.0302 (5)	0.0194 (4)	0.0160 (4)	0.0103 (4)	0.0069 (4)	−0.0002 (3)
O2B	0.0276 (5)	0.0161 (4)	0.0166 (4)	0.0066 (3)	0.0050 (3)	0.0004 (3)
C1B	0.0156 (5)	0.0128 (4)	0.0175 (5)	0.0005 (4)	0.0053 (4)	−0.0010 (4)
C2B	0.0149 (5)	0.0140 (5)	0.0154 (5)	0.0015 (4)	0.0045 (4)	−0.0008 (4)
C3B	0.0204 (6)	0.0197 (5)	0.0149 (5)	0.0038 (4)	0.0027 (4)	0.0001 (4)
C4B	0.0203 (6)	0.0186 (5)	0.0197 (6)	0.0067 (4)	0.0014 (4)	0.0033 (4)
C5B	0.0136 (5)	0.0144 (5)	0.0205 (5)	0.0028 (4)	0.0034 (4)	0.0001 (4)
C6B	0.0210 (6)	0.0191 (5)	0.0305 (7)	0.0051 (5)	0.0078 (5)	−0.0050 (5)

Geometric parameters (Å, º)

Cl1—C5A	1.7293 (11)	C8A—H8A3	0.9800
N1A—C2A	1.3331 (14)	C8A—H8A4	0.9800
N1A—C6A	1.3603 (15)	C8A—H8A5	0.9800
C2A—N3A	1.3421 (14)	C8A—H8A6	0.9800
C2A—C7A	1.5007 (16)	S1—C5B	1.7163 (12)
N3A—C4A	1.3528 (14)	S1—C2B	1.7199 (12)
N4A—C4A	1.3340 (14)	O1B—C1B	1.3180 (15)
N4A—H41	0.86 (2)	O1B—H1B	0.92 (2)
N4A—H42	0.842 (19)	O2B—C1B	1.2232 (15)
C4A—C5A	1.4175 (15)	C1B—C2B	1.4732 (16)
C5A—C6A	1.3753 (15)	C2B—C3B	1.3706 (16)
C6A—C8A	1.5013 (15)	C3B—C4B	1.4215 (17)
C7A—H7A1	0.9800	C3B—H3BA	0.9500
C7A—H7A2	0.9800	C4B—C5B	1.3712 (18)
C7A—H7A3	0.9800	C4B—H4BA	0.9500
C7A—H7A4	0.9800	C5B—C6B	1.4994 (17)
C7A—H7A5	0.9800	C6B—H6BA	0.9800
C7A—H7A6	0.9800	C6B—H6BB	0.9800
C8A—H8A1	0.9800	C6B—H6BC	0.9800

C8A—H8A2	0.9800		
C2A—N1A—C6A	116.94 (10)	C6A—C8A—H8A3	109.5
N1A—C2A—N3A	125.97 (10)	H8A1—C8A—H8A3	109.5
N1A—C2A—C7A	117.79 (10)	H8A2—C8A—H8A3	109.5
N3A—C2A—C7A	116.23 (10)	C6A—C8A—H8A4	109.5
C2A—N3A—C4A	118.30 (9)	H8A1—C8A—H8A4	141.1
C4A—N4A—H41	120.2 (13)	H8A2—C8A—H8A4	56.3
C4A—N4A—H42	116.7 (12)	H8A3—C8A—H8A4	56.3
H41—N4A—H42	122.8 (18)	C6A—C8A—H8A5	109.5
N4A—C4A—N3A	118.61 (10)	H8A1—C8A—H8A5	56.3
N4A—C4A—C5A	122.91 (10)	H8A2—C8A—H8A5	141.1
N3A—C4A—C5A	118.48 (10)	H8A3—C8A—H8A5	56.3
C6A—C5A—C4A	119.53 (10)	H8A4—C8A—H8A5	109.5
C6A—C5A—Cl1	121.95 (9)	C6A—C8A—H8A6	109.5
C4A—C5A—Cl1	118.52 (8)	H8A1—C8A—H8A6	56.3
N1A—C6A—C5A	120.68 (10)	H8A2—C8A—H8A6	56.3
N1A—C6A—C8A	116.90 (10)	H8A3—C8A—H8A6	141.1
C5A—C6A—C8A	122.42 (10)	H8A4—C8A—H8A6	109.5
C2A—C7A—H7A1	109.5	H8A5—C8A—H8A6	109.5
C2A—C7A—H7A2	109.5	C5B—S1—C2B	92.42 (6)
H7A1—C7A—H7A2	109.5	C1B—O1B—H1B	111.3 (13)
C2A—C7A—H7A3	109.5	O2B—C1B—O1B	124.53 (11)
H7A1—C7A—H7A3	109.5	O2B—C1B—C2B	122.02 (11)
H7A2—C7A—H7A3	109.5	O1B—C1B—C2B	113.46 (10)
C2A—C7A—H7A4	109.5	C3B—C2B—C1B	129.64 (11)
H7A1—C7A—H7A4	141.1	C3B—C2B—S1	111.17 (9)
H7A2—C7A—H7A4	56.3	C1B—C2B—S1	119.18 (9)
H7A3—C7A—H7A4	56.3	C2B—C3B—C4B	112.46 (11)
C2A—C7A—H7A5	109.5	C2B—C3B—H3BA	123.8
H7A1—C7A—H7A5	56.3	C4B—C3B—H3BA	123.8
H7A2—C7A—H7A5	141.1	C5B—C4B—C3B	112.98 (11)
H7A3—C7A—H7A5	56.3	C5B—C4B—H4BA	123.5
H7A4—C7A—H7A5	109.5	C3B—C4B—H4BA	123.5
C2A—C7A—H7A6	109.5	C4B—C5B—C6B	128.60 (11)
H7A1—C7A—H7A6	56.3	C4B—C5B—S1	110.96 (9)
H7A2—C7A—H7A6	56.3	C6B—C5B—S1	120.44 (10)
H7A3—C7A—H7A6	141.1	C5B—C6B—H6BA	109.5
H7A4—C7A—H7A6	109.5	C5B—C6B—H6BB	109.5
H7A5—C7A—H7A6	109.5	H6BA—C6B—H6BB	109.5
C6A—C8A—H8A1	109.5	C5B—C6B—H6BC	109.5
C6A—C8A—H8A2	109.5	H6BA—C6B—H6BC	109.5
H8A1—C8A—H8A2	109.5	H6BB—C6B—H6BC	109.5
C6A—N1A—C2A—N3A	2.31 (17)	Cl1—C5A—C6A—C8A	−1.57 (15)
C6A—N1A—C2A—C7A	−177.41 (10)	O2B—C1B—C2B—C3B	−179.21 (12)
N1A—C2A—N3A—C4A	−0.18 (17)	O1B—C1B—C2B—C3B	0.46 (18)
C7A—C2A—N3A—C4A	179.55 (10)	O2B—C1B—C2B—S1	−0.45 (16)

C2A—N3A—C4A—N4A	177.78 (10)	O1B—C1B—C2B—S1	179.21 (9)
C2A—N3A—C4A—C5A	−2.41 (15)	C5B—S1—C2B—C3B	−0.20 (10)
N4A—C4A—C5A—C6A	−177.34 (11)	C5B—S1—C2B—C1B	−179.17 (10)
N3A—C4A—C5A—C6A	2.85 (16)	C1B—C2B—C3B—C4B	178.92 (12)
N4A—C4A—C5A—Cl1	3.19 (15)	S1—C2B—C3B—C4B	0.09 (14)
N3A—C4A—C5A—Cl1	−176.62 (8)	C2B—C3B—C4B—C5B	0.11 (17)
C2A—N1A—C6A—C5A	−1.75 (16)	C3B—C4B—C5B—C6B	−179.99 (12)
C2A—N1A—C6A—C8A	178.53 (10)	C3B—C4B—C5B—S1	−0.25 (15)
C4A—C5A—C6A—N1A	−0.72 (16)	C2B—S1—C5B—C4B	0.26 (10)
Cl1—C5A—C6A—N1A	178.72 (8)	C2B—S1—C5B—C6B	−179.98 (10)
C4A—C5A—C6A—C8A	178.98 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4*A*—H41···N1*A*^{i}	0.86 (2)	2.27 (2)	3.0790 (16)	158.0 (18)
N4*A*—H42···O2*B*	0.842 (19)	2.065 (19)	2.9028 (15)	173.6 (18)
O1*B*—H1*B*···N3*A*	0.92 (2)	1.74 (2)	2.6607 (14)	173 (2)

Symmetry code: (i) x, $-y+3/2$, $z-1/2$.

4-Amino-5-chloro-2,6-dimethylpyrimidine–benzoic acid (1/1) (COCRYSTAL-6)

Crystal data

$C_6H_8ClN_3·C_7H_6O_2$
M_r = 279.72
Monoclinic, $P2_1/c$
a = 10.1421 (5) Å
b = 10.4218 (5) Å
c = 13.2681 (6) Å
β = 107.804 (5)°
V = 1335.26 (12) Å^3
Z = 4
$F(000)$ = 584
D_x = 1.391 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 2966 reflections
θ = 4.2–76.3°
μ = 2.56 mm^{-1}
T = 120 K
Chunk, colorless
0.52 × 0.38 × 0.24 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: sealed X-ray tube
Detector resolution: 10.6501 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.763, T_{max} = 1.000
6087 measured reflections
2760 independent reflections
2560 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 76.6°, θ_{min} = 4.6°
h = −12→12
k = −9→12
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.118
S = 1.04
2760 reflections
187 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0793P)^2 + 0.3948P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Extinction correction: SHELXL2014 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0032 (7)

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.39577 (4)	0.14749 (3)	0.34668 (3)	0.02536 (16)
N1A	0.54933 (13)	0.30904 (13)	0.63034 (9)	0.0215 (3)
C2A	0.63967 (14)	0.38934 (15)	0.60876 (11)	0.0204 (3)
N3A	0.66375 (12)	0.40143 (12)	0.51529 (9)	0.0201 (3)
N4A	0.61835 (15)	0.33300 (14)	0.34212 (10)	0.0241 (3)
H41	0.682 (2)	0.386 (2)	0.3405 (16)	0.028 (5)*
H42	0.583 (2)	0.273 (2)	0.2896 (17)	0.030 (5)*
C4A	0.59268 (15)	0.32453 (14)	0.43453 (11)	0.0196 (3)
C5A	0.49274 (15)	0.23975 (14)	0.45181 (11)	0.0208 (3)
C6A	0.47284 (15)	0.23477 (15)	0.54949 (12)	0.0214 (3)
C7A	0.72207 (17)	0.47425 (16)	0.69690 (12)	0.0266 (3)
H7AA	0.6936	0.4592	0.7601	0.040*
H7AB	0.7056	0.5643	0.6754	0.040*
H7AC	0.8208	0.4547	0.7127	0.040*
C8A	0.36724 (17)	0.14862 (16)	0.57215 (13)	0.0277 (4)
H8AA	0.3599	0.1683	0.6425	0.042*
H8AB	0.3955	0.0590	0.5701	0.042*
H8AC	0.2772	0.1622	0.5187	0.042*
O1B	0.81428 (11)	0.52642 (10)	0.33828 (8)	0.0236 (3)
O2B	0.84927 (12)	0.58025 (11)	0.50792 (8)	0.0261 (3)
H2B	0.787 (3)	0.521 (2)	0.5057 (18)	0.040 (6)*
C1B	0.96195 (14)	0.70251 (14)	0.40863 (12)	0.0207 (3)
C2B	1.03036 (16)	0.77548 (16)	0.49703 (12)	0.0271 (3)
H2BA	1.0184	0.7568	0.5638	0.032*
C3B	1.11636 (19)	0.87588 (18)	0.48757 (14)	0.0322 (4)
H3BA	1.1636	0.9253	0.5480	0.039*
C4B	1.13303 (18)	0.90380 (17)	0.38984 (14)	0.0307 (4)
H4BA	1.1919	0.9722	0.3835	0.037*
C5B	1.06404 (19)	0.83225 (18)	0.30168 (14)	0.0317 (4)
H5BA	1.0750	0.8521	0.2348	0.038*
C6B	0.97869 (17)	0.73133 (16)	0.31075 (12)	0.0272 (3)
H6BA	0.9318	0.6820	0.2502	0.033*
C7B	0.86845 (14)	0.59440 (14)	0.41483 (11)	0.0200 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0262 (2)	0.0295 (2)	0.0204 (2)	−0.00904 (13)	0.00707 (15)	−0.00331 (12)
N1A	0.0225 (6)	0.0257 (7)	0.0168 (6)	−0.0013 (5)	0.0069 (5)	0.0004 (5)
C2A	0.0209 (7)	0.0233 (7)	0.0180 (6)	0.0017 (6)	0.0073 (5)	0.0011 (6)
N3A	0.0205 (6)	0.0230 (6)	0.0175 (6)	−0.0014 (5)	0.0069 (5)	−0.0008 (5)
N4A	0.0270 (7)	0.0298 (7)	0.0175 (6)	−0.0099 (6)	0.0097 (5)	−0.0038 (5)
C4A	0.0186 (6)	0.0226 (7)	0.0179 (7)	0.0007 (5)	0.0061 (5)	0.0003 (5)
C5A	0.0201 (7)	0.0233 (7)	0.0190 (7)	−0.0022 (5)	0.0058 (5)	0.0001 (5)
C6A	0.0199 (7)	0.0237 (7)	0.0214 (7)	0.0003 (5)	0.0073 (5)	0.0026 (6)
C7A	0.0300 (8)	0.0303 (8)	0.0196 (7)	−0.0042 (6)	0.0079 (6)	−0.0038 (6)
C8A	0.0271 (8)	0.0331 (9)	0.0255 (8)	−0.0078 (6)	0.0119 (7)	0.0017 (6)
O1B	0.0252 (5)	0.0249 (6)	0.0220 (5)	−0.0050 (4)	0.0092 (4)	−0.0015 (4)
O2B	0.0303 (6)	0.0296 (6)	0.0204 (5)	−0.0098 (5)	0.0109 (4)	−0.0009 (4)
C1B	0.0188 (6)	0.0213 (7)	0.0226 (7)	−0.0003 (5)	0.0073 (5)	0.0020 (6)
C2B	0.0296 (8)	0.0302 (8)	0.0210 (7)	−0.0069 (6)	0.0070 (6)	−0.0004 (6)
C3B	0.0346 (9)	0.0332 (9)	0.0270 (8)	−0.0126 (7)	0.0068 (7)	−0.0021 (7)
C4B	0.0312 (8)	0.0290 (8)	0.0330 (8)	−0.0094 (7)	0.0111 (7)	0.0014 (7)
C5B	0.0375 (9)	0.0347 (9)	0.0263 (8)	−0.0102 (7)	0.0148 (7)	0.0010 (7)
C6B	0.0306 (8)	0.0303 (8)	0.0228 (7)	−0.0073 (7)	0.0113 (6)	−0.0019 (6)
C7B	0.0180 (6)	0.0224 (7)	0.0203 (7)	0.0018 (5)	0.0070 (5)	0.0020 (5)

Geometric parameters (Å, º)

Cl1—C5A	1.7316 (15)	C8A—H8AC	0.9800
N1A—C2A	1.335 (2)	O1B—C7B	1.2224 (18)
N1A—C6A	1.357 (2)	O2B—C7B	1.3160 (18)
C2A—N3A	1.3411 (18)	O2B—H2B	0.87 (3)
C2A—C7A	1.500 (2)	C1B—C2B	1.392 (2)
N3A—C4A	1.3557 (19)	C1B—C6B	1.393 (2)
N4A—C4A	1.3320 (19)	C1B—C7B	1.491 (2)
N4A—H41	0.86 (2)	C2B—C3B	1.392 (2)
N4A—H42	0.92 (2)	C2B—H2BA	0.9500
C4A—C5A	1.415 (2)	C3B—C4B	1.389 (2)
C5A—C6A	1.372 (2)	C3B—H3BA	0.9500
C6A—C8A	1.497 (2)	C4B—C5B	1.383 (2)
C7A—H7AA	0.9800	C4B—H4BA	0.9500
C7A—H7AB	0.9800	C5B—C6B	1.391 (2)
C7A—H7AC	0.9800	C5B—H5BA	0.9500
C8A—H8AA	0.9800	C6B—H6BA	0.9500
C8A—H8AB	0.9800		
C2A—N1A—C6A	116.86 (12)	C6A—C8A—H8AC	109.5
N1A—C2A—N3A	126.03 (14)	H8AA—C8A—H8AC	109.5
N1A—C2A—C7A	117.24 (12)	H8AB—C8A—H8AC	109.5
N3A—C2A—C7A	116.73 (13)	C7B—O2B—H2B	111.1 (15)
C2A—N3A—C4A	118.18 (12)	C2B—C1B—C6B	119.75 (14)

C4A—N4A—H41	115.3 (14)	C2B—C1B—C7B	121.87 (13)
C4A—N4A—H42	120.6 (13)	C6B—C1B—C7B	118.37 (13)
H41—N4A—H42	122.8 (19)	C1B—C2B—C3B	119.95 (15)
N4A—C4A—N3A	118.82 (13)	C1B—C2B—H2BA	120.0
N4A—C4A—C5A	122.81 (14)	C3B—C2B—H2BA	120.0
N3A—C4A—C5A	118.36 (13)	C4B—C3B—C2B	120.00 (16)
C6A—C5A—C4A	119.74 (13)	C4B—C3B—H3BA	120.0
C6A—C5A—Cl1	121.90 (11)	C2B—C3B—H3BA	120.0
C4A—C5A—Cl1	118.34 (11)	C5B—C4B—C3B	120.14 (15)
N1A—C6A—C5A	120.74 (13)	C5B—C4B—H4BA	119.9
N1A—C6A—C8A	117.03 (13)	C3B—C4B—H4BA	119.9
C5A—C6A—C8A	122.23 (14)	C4B—C5B—C6B	120.12 (15)
C2A—C7A—H7AA	109.5	C4B—C5B—H5BA	119.9
C2A—C7A—H7AB	109.5	C6B—C5B—H5BA	119.9
H7AA—C7A—H7AB	109.5	C5B—C6B—C1B	120.02 (15)
C2A—C7A—H7AC	109.5	C5B—C6B—H6BA	120.0
H7AA—C7A—H7AC	109.5	C1B—C6B—H6BA	120.0
H7AB—C7A—H7AC	109.5	O1B—C7B—O2B	123.85 (13)
C6A—C8A—H8AA	109.5	O1B—C7B—C1B	121.60 (13)
C6A—C8A—H8AB	109.5	O2B—C7B—C1B	114.54 (13)
H8AA—C8A—H8AB	109.5		

C6A—N1A—C2A—N3A	−1.5 (2)	C4A—C5A—C6A—C8A	179.03 (14)
C6A—N1A—C2A—C7A	178.46 (13)	Cl1—C5A—C6A—C8A	0.6 (2)
N1A—C2A—N3A—C4A	−1.2 (2)	C6B—C1B—C2B—C3B	−0.7 (2)
C7A—C2A—N3A—C4A	178.89 (13)	C7B—C1B—C2B—C3B	−179.78 (15)
C2A—N3A—C4A—N4A	−178.15 (14)	C1B—C2B—C3B—C4B	0.5 (3)
C2A—N3A—C4A—C5A	2.7 (2)	C2B—C3B—C4B—C5B	0.2 (3)
N4A—C4A—C5A—C6A	179.16 (14)	C3B—C4B—C5B—C6B	−0.6 (3)
N3A—C4A—C5A—C6A	−1.7 (2)	C4B—C5B—C6B—C1B	0.3 (3)
N4A—C4A—C5A—Cl1	−2.3 (2)	C2B—C1B—C6B—C5B	0.3 (2)
N3A—C4A—C5A—Cl1	176.75 (11)	C7B—C1B—C6B—C5B	179.40 (15)
C2A—N1A—C6A—C5A	2.5 (2)	C2B—C1B—C7B—O1B	−176.15 (14)
C2A—N1A—C6A—C8A	−177.49 (13)	C6B—C1B—C7B—O1B	4.8 (2)
C4A—C5A—C6A—N1A	−0.9 (2)	C2B—C1B—C7B—O2B	4.4 (2)
Cl1—C5A—C6A—N1A	−179.35 (11)	C6B—C1B—C7B—O2B	−174.61 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4*A*—H41···O1*B*	0.86 (2)	1.99 (2)	2.8419 (17)	173 (2)
N4*A*—H42···N1*A*^{i}	0.92 (2)	2.21 (2)	3.0617 (18)	153.5 (18)
C8*A*—H8*AB*···Cl1^{ii}	0.98	2.98	3.8571 (18)	149
O2*B*—H2*B*···N3*A*	0.87 (3)	1.80 (3)	2.6712 (17)	174 (2)

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

4-Amino-5-chloro-2,6-dimethylpyrimidine–2-methylbenzoic acid (1/1) (COCRYSTAL-7)

Crystal data

$C_6H_8ClN_3 \cdot C_8H_8O_2$
$M_r = 293.75$
Orthorhombic, $P2_12_12_1$
$a = 7.3992$ (2) Å
$b = 13.9842$ (4) Å
$c = 26.9897$ (8) Å
$V = 2792.68$ (14) Å^3
$Z = 8$
$F(000) = 1232$
$D_x = 1.397$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 3914 reflections
$\theta = 3.6$–$76.5°$
$\mu = 2.47$ mm^{-1}
$T = 120$ K
Needle, colorless
0.49 × 0.11 × 0.08 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: sealed X-ray tube
Detector resolution: 10.6501 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
$T_{min} = 0.740$, $T_{max} = 1.000$
8897 measured reflections
4966 independent reflections
4617 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 76.8°$, $\theta_{min} = 3.3°$
$h = -7 \rightarrow 9$
$k = -17 \rightarrow 14$
$l = -22 \rightarrow 34$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.091$
$S = 1.04$
4966 reflections
376 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 0.3891P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00039 (10)
Absolute structure: Flack x determined using 1451 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.001 (10)

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.91235 (8)	0.87398 (4)	0.43040 (2)	0.02206 (15)
N1A	0.7729 (3)	1.10678 (15)	0.50704 (8)	0.0201 (4)
C2A	0.7196 (4)	1.06463 (18)	0.54874 (9)	0.0192 (5)
N3A	0.7172 (3)	0.97006 (15)	0.55756 (8)	0.0191 (4)
N4A	0.7653 (4)	0.81632 (16)	0.53005 (8)	0.0234 (5)
H4AA	0.7255	0.7950	0.5587	0.028*

H4AB	0.8004	0.7757	0.5071	0.028*
C4A	0.7723 (4)	0.91023 (18)	0.52138 (9)	0.0183 (5)
C5A	0.8346 (4)	0.95017 (19)	0.47634 (9)	0.0185 (5)
C6A	0.8313 (4)	1.0482 (2)	0.47023 (10)	0.0204 (5)
C7A	0.6540 (4)	1.12797 (19)	0.58987 (9)	0.0231 (5)
H7AA	0.7146	1.1902	0.5878	0.035*
H7AB	0.6814	1.0982	0.6219	0.035*
H7AC	0.5231	1.1370	0.5868	0.035*
C8A	0.8890 (4)	1.0961 (2)	0.42303 (10)	0.0258 (6)
H8AA	0.9284	1.1616	0.4302	0.039*
H8AB	0.7871	1.0978	0.3999	0.039*
H8AC	0.9892	1.0603	0.4082	0.039*
Cl2	0.88558 (8)	0.36846 (4)	0.56903 (2)	0.02260 (15)
N1B	0.7984 (3)	0.60749 (15)	0.49210 (8)	0.0203 (4)
C2B	0.7345 (4)	0.56860 (18)	0.45060 (9)	0.0186 (5)
N3B	0.7075 (3)	0.47481 (15)	0.44219 (8)	0.0190 (4)
N4B	0.7245 (4)	0.31988 (16)	0.46998 (8)	0.0231 (5)
H4BA	0.6796	0.3010	0.4414	0.028*
H4BB	0.7517	0.2775	0.4929	0.028*
C4B	0.7514 (4)	0.41261 (18)	0.47854 (9)	0.0190 (5)
C5B	0.8238 (4)	0.44877 (19)	0.52313 (9)	0.0186 (5)
C6B	0.8434 (3)	0.54633 (19)	0.52929 (9)	0.0190 (5)
C7B	0.6863 (4)	0.63491 (19)	0.40878 (10)	0.0250 (5)
H7BA	0.6899	0.7012	0.4205	0.037*
H7BB	0.5645	0.6200	0.3968	0.037*
H7BC	0.7732	0.6268	0.3817	0.037*
C8B	0.9118 (4)	0.59057 (19)	0.57601 (10)	0.0238 (5)
H8BA	0.9847	0.6470	0.5680	0.036*
H8BB	0.9864	0.5441	0.5939	0.036*
H8BC	0.8094	0.6096	0.5968	0.036*
O1C	0.6542 (4)	0.92635 (14)	0.65200 (7)	0.0346 (6)
H1C	0.675 (7)	0.938 (4)	0.6173 (19)	0.071 (16)*
O2C	0.6384 (3)	0.77291 (14)	0.63071 (7)	0.0288 (5)
C1C	0.5787 (4)	0.81731 (18)	0.71489 (9)	0.0191 (5)
C2C	0.5895 (4)	0.72517 (18)	0.73568 (9)	0.0195 (5)
C3C	0.5330 (4)	0.71465 (18)	0.78504 (9)	0.0217 (5)
H3CA	0.5403	0.6535	0.8002	0.026*
C4C	0.4672 (4)	0.7903 (2)	0.81212 (9)	0.0245 (5)
H4CA	0.4281	0.7805	0.8453	0.029*
C5C	0.4574 (4)	0.88148 (19)	0.79126 (10)	0.0239 (5)
H5CA	0.4119	0.9339	0.8098	0.029*
C6C	0.5155 (4)	0.89400 (17)	0.74291 (9)	0.0213 (5)
H6CA	0.5121	0.9560	0.7286	0.026*
C7C	0.6283 (4)	0.83490 (18)	0.66198 (10)	0.0205 (5)
C8C	0.6594 (4)	0.63891 (18)	0.70853 (10)	0.0228 (5)
H8CA	0.7754	0.6544	0.6930	0.034*
H8CB	0.5723	0.6200	0.6830	0.034*
H8CC	0.6759	0.5861	0.7320	0.034*

O1D	0.5864 (3)	0.43696 (13)	0.35050 (7)	0.0299 (5)
H1D	0.633 (6)	0.443 (3)	0.3830 (16)	0.049 (12)*
O2D	0.5744 (3)	0.28307 (13)	0.37102 (7)	0.0258 (4)
C1D	0.4706 (4)	0.33139 (18)	0.29067 (9)	0.0187 (5)
C2D	0.4639 (4)	0.23980 (18)	0.26889 (9)	0.0206 (5)
C3D	0.3967 (4)	0.23334 (19)	0.22030 (10)	0.0224 (5)
H3DA	0.3961	0.1729	0.2042	0.027*
C4D	0.3317 (4)	0.3120 (2)	0.19525 (10)	0.0246 (5)
H4DA	0.2858	0.3050	0.1626	0.029*
C5D	0.3330 (4)	0.40158 (19)	0.21763 (10)	0.0242 (5)
H5DA	0.2869	0.4558	0.2006	0.029*
C6D	0.4023 (4)	0.41093 (18)	0.26514 (10)	0.0209 (5)
H6DA	0.4036	0.4720	0.2806	0.025*
C7D	0.5482 (4)	0.34623 (18)	0.34092 (9)	0.0198 (5)
C8D	0.5261 (4)	0.14993 (18)	0.29421 (10)	0.0250 (6)
H8DA	0.5127	0.0956	0.2715	0.037*
H8DB	0.4529	0.1390	0.3239	0.037*
H8DC	0.6534	0.1566	0.3037	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0255 (3)	0.0205 (3)	0.0201 (3)	0.0010 (2)	0.0027 (2)	−0.0043 (2)
N1A	0.0225 (11)	0.0162 (10)	0.0217 (9)	−0.0022 (9)	0.0007 (9)	0.0010 (8)
C2A	0.0203 (12)	0.0162 (12)	0.0211 (11)	−0.0015 (10)	−0.0003 (10)	−0.0003 (9)
N3A	0.0231 (10)	0.0153 (10)	0.0190 (9)	−0.0012 (9)	0.0020 (8)	−0.0005 (8)
N4A	0.0345 (13)	0.0151 (10)	0.0207 (9)	−0.0004 (10)	0.0053 (10)	−0.0011 (8)
C4A	0.0196 (12)	0.0148 (11)	0.0206 (11)	0.0015 (10)	−0.0021 (10)	−0.0010 (9)
C5A	0.0200 (12)	0.0188 (12)	0.0168 (10)	0.0004 (10)	0.0008 (10)	−0.0023 (10)
C6A	0.0197 (12)	0.0209 (12)	0.0204 (11)	0.0014 (11)	0.0004 (10)	0.0002 (10)
C7A	0.0301 (13)	0.0165 (11)	0.0227 (11)	0.0000 (11)	0.0038 (11)	−0.0013 (10)
C8A	0.0303 (13)	0.0241 (12)	0.0231 (12)	0.0008 (12)	0.0052 (12)	0.0042 (11)
Cl2	0.0268 (3)	0.0200 (3)	0.0210 (3)	0.0018 (2)	−0.0034 (2)	0.0040 (2)
N1B	0.0237 (11)	0.0161 (9)	0.0212 (9)	0.0016 (9)	−0.0007 (9)	−0.0019 (8)
C2B	0.0215 (12)	0.0141 (11)	0.0202 (11)	0.0021 (10)	0.0012 (10)	−0.0005 (9)
N3B	0.0242 (10)	0.0153 (10)	0.0175 (9)	0.0003 (9)	0.0006 (8)	−0.0007 (8)
N4B	0.0333 (12)	0.0149 (9)	0.0211 (9)	−0.0012 (10)	−0.0050 (10)	0.0009 (8)
C4B	0.0205 (12)	0.0161 (11)	0.0204 (11)	0.0008 (10)	0.0035 (10)	0.0000 (9)
C5B	0.0204 (12)	0.0165 (11)	0.0188 (11)	0.0041 (10)	0.0001 (10)	0.0006 (10)
C6B	0.0178 (12)	0.0194 (12)	0.0199 (11)	0.0023 (10)	0.0002 (10)	−0.0015 (10)
C7B	0.0348 (14)	0.0166 (11)	0.0235 (11)	−0.0006 (12)	−0.0045 (11)	0.0028 (10)
C8B	0.0255 (13)	0.0215 (12)	0.0244 (12)	0.0018 (11)	−0.0060 (11)	−0.0050 (10)
O1C	0.0660 (17)	0.0175 (9)	0.0202 (9)	−0.0079 (10)	0.0104 (10)	−0.0017 (7)
O2C	0.0468 (13)	0.0190 (9)	0.0206 (8)	−0.0022 (9)	0.0030 (9)	−0.0005 (7)
C1C	0.0196 (12)	0.0166 (11)	0.0211 (11)	−0.0019 (10)	−0.0006 (10)	−0.0001 (9)
C2C	0.0200 (12)	0.0173 (11)	0.0211 (11)	−0.0024 (11)	−0.0010 (10)	0.0004 (9)
C3C	0.0257 (13)	0.0173 (11)	0.0221 (11)	−0.0039 (11)	−0.0018 (11)	0.0037 (9)
C4C	0.0281 (13)	0.0269 (13)	0.0186 (11)	−0.0054 (12)	0.0015 (11)	0.0003 (10)

C5C	0.0284 (13)	0.0211 (12)	0.0222 (11)	−0.0011 (11)	0.0030 (11)	−0.0029 (10)
C6C	0.0257 (13)	0.0156 (10)	0.0227 (11)	−0.0017 (10)	−0.0008 (11)	0.0019 (10)
C7C	0.0227 (12)	0.0168 (11)	0.0218 (11)	−0.0034 (10)	−0.0005 (10)	0.0014 (9)
C8C	0.0276 (13)	0.0149 (11)	0.0260 (12)	−0.0016 (11)	0.0011 (11)	0.0013 (10)
O1D	0.0491 (13)	0.0156 (8)	0.0250 (9)	−0.0055 (9)	−0.0112 (10)	−0.0004 (7)
O2D	0.0385 (11)	0.0180 (8)	0.0208 (8)	−0.0034 (9)	−0.0039 (9)	0.0012 (7)
C1D	0.0198 (12)	0.0175 (11)	0.0186 (10)	−0.0012 (10)	0.0005 (10)	−0.0001 (9)
C2D	0.0218 (13)	0.0184 (11)	0.0215 (11)	−0.0002 (10)	0.0015 (10)	−0.0004 (9)
C3D	0.0236 (13)	0.0213 (12)	0.0222 (12)	−0.0030 (11)	0.0010 (10)	−0.0057 (10)
C4D	0.0235 (13)	0.0287 (13)	0.0215 (11)	−0.0035 (11)	−0.0031 (11)	0.0001 (10)
C5D	0.0249 (13)	0.0210 (12)	0.0266 (12)	−0.0006 (11)	−0.0034 (11)	0.0046 (10)
C6D	0.0228 (12)	0.0153 (10)	0.0246 (12)	−0.0016 (11)	0.0013 (11)	−0.0010 (9)
C7D	0.0219 (11)	0.0173 (11)	0.0203 (11)	−0.0019 (10)	0.0021 (10)	−0.0026 (9)
C8D	0.0320 (14)	0.0170 (11)	0.0258 (12)	0.0019 (11)	−0.0012 (11)	−0.0024 (10)

Geometric parameters (Å, º)

Cl1—C5A	1.733 (3)	O1C—C7C	1.321 (3)
N1A—C2A	1.330 (3)	O1C—H1C	0.96 (5)
N1A—C6A	1.359 (3)	O2C—C7C	1.212 (3)
C2A—N3A	1.344 (3)	C1C—C6C	1.393 (4)
C2A—C7A	1.501 (4)	C1C—C2C	1.408 (3)
N3A—C4A	1.349 (3)	C1C—C7C	1.495 (3)
N4A—C4A	1.335 (3)	C2C—C3C	1.404 (3)
N4A—H4AA	0.8800	C2C—C8C	1.503 (4)
N4A—H4AB	0.8800	C3C—C4C	1.375 (4)
C4A—C5A	1.415 (4)	C3C—H3CA	0.9500
C5A—C6A	1.380 (4)	C4C—C5C	1.395 (4)
C6A—C8A	1.502 (4)	C4C—H4CA	0.9500
C7A—H7AA	0.9800	C5C—C6C	1.385 (4)
C7A—H7AB	0.9800	C5C—H5CA	0.9500
C7A—H7AC	0.9800	C6C—H6CA	0.9500
C8A—H8AA	0.9800	C8C—H8CA	0.9800
C8A—H8AB	0.9800	C8C—H8CB	0.9800
C8A—H8AC	0.9800	C8C—H8CC	0.9800
Cl2—C5B	1.734 (3)	O1D—C7D	1.325 (3)
N1B—C2B	1.332 (3)	O1D—H1D	0.95 (4)
N1B—C6B	1.360 (3)	O2D—C7D	1.216 (3)
C2B—N3B	1.346 (3)	C1D—C6D	1.402 (4)
C2B—C7B	1.504 (3)	C1D—C2D	1.410 (4)
N3B—C4B	1.351 (3)	C1D—C7D	1.487 (3)
N4B—C4B	1.332 (3)	C2D—C3D	1.406 (4)
N4B—H4BA	0.8800	C2D—C8D	1.503 (4)
N4B—H4BB	0.8800	C3D—C4D	1.378 (4)
C4B—C5B	1.411 (4)	C3D—H3DA	0.9500
C5B—C6B	1.382 (4)	C4D—C5D	1.391 (4)
C6B—C8B	1.493 (3)	C4D—H4DA	0.9500
C7B—H7BA	0.9800	C5D—C6D	1.387 (4)

C7B—H7BB	0.9800	C5D—H5DA	0.9500
C7B—H7BC	0.9800	C6D—H6DA	0.9500
C8B—H8BA	0.9800	C8D—H8DA	0.9800
C8B—H8BB	0.9800	C8D—H8DB	0.9800
C8B—H8BC	0.9800	C8D—H8DC	0.9800
C2A—N1A—C6A	116.5 (2)	H8BB—C8B—H8BC	109.5
N1A—C2A—N3A	126.1 (2)	C7C—O1C—H1C	112 (3)
N1A—C2A—C7A	117.4 (2)	C6C—C1C—C2C	120.5 (2)
N3A—C2A—C7A	116.5 (2)	C6C—C1C—C7C	118.3 (2)
C2A—N3A—C4A	118.6 (2)	C2C—C1C—C7C	121.2 (2)
C4A—N4A—H4AA	120.0	C3C—C2C—C1C	117.2 (2)
C4A—N4A—H4AB	120.0	C3C—C2C—C8C	118.7 (2)
H4AA—N4A—H4AB	120.0	C1C—C2C—C8C	124.1 (2)
N4A—C4A—N3A	118.1 (2)	C4C—C3C—C2C	121.9 (2)
N4A—C4A—C5A	123.5 (2)	C4C—C3C—H3CA	119.0
N3A—C4A—C5A	118.4 (2)	C2C—C3C—H3CA	119.0
C6A—C5A—C4A	119.3 (2)	C3C—C4C—C5C	120.5 (2)
C6A—C5A—Cl1	122.06 (19)	C3C—C4C—H4CA	119.8
C4A—C5A—Cl1	118.7 (2)	C5C—C4C—H4CA	119.8
N1A—C6A—C5A	121.2 (2)	C6C—C5C—C4C	118.7 (3)
N1A—C6A—C8A	116.2 (2)	C6C—C5C—H5CA	120.7
C5A—C6A—C8A	122.7 (2)	C4C—C5C—H5CA	120.7
C2A—C7A—H7AA	109.5	C5C—C6C—C1C	121.2 (2)
C2A—C7A—H7AB	109.5	C5C—C6C—H6CA	119.4
H7AA—C7A—H7AB	109.5	C1C—C6C—H6CA	119.4
C2A—C7A—H7AC	109.5	O2C—C7C—O1C	122.8 (2)
H7AA—C7A—H7AC	109.5	O2C—C7C—C1C	124.2 (2)
H7AB—C7A—H7AC	109.5	O1C—C7C—C1C	112.9 (2)
C6A—C8A—H8AA	109.5	C2C—C8C—H8CA	109.5
C6A—C8A—H8AB	109.5	C2C—C8C—H8CB	109.5
H8AA—C8A—H8AB	109.5	H8CA—C8C—H8CB	109.5
C6A—C8A—H8AC	109.5	C2C—C8C—H8CC	109.5
H8AA—C8A—H8AC	109.5	H8CA—C8C—H8CC	109.5
H8AB—C8A—H8AC	109.5	H8CB—C8C—H8CC	109.5
C2B—N1B—C6B	116.8 (2)	C7D—O1D—H1D	110 (3)
N1B—C2B—N3B	126.3 (2)	C6D—C1D—C2D	120.2 (2)
N1B—C2B—C7B	117.6 (2)	C6D—C1D—C7D	118.4 (2)
N3B—C2B—C7B	116.1 (2)	C2D—C1D—C7D	121.3 (2)
C2B—N3B—C4B	118.0 (2)	C3D—C2D—C1D	117.4 (2)
C4B—N4B—H4BA	120.0	C3D—C2D—C8D	118.6 (2)
C4B—N4B—H4BB	120.0	C1D—C2D—C8D	124.0 (2)
H4BA—N4B—H4BB	120.0	C4D—C3D—C2D	122.0 (2)
N4B—C4B—N3B	117.7 (2)	C4D—C3D—H3DA	119.0
N4B—C4B—C5B	123.6 (2)	C2D—C3D—H3DA	119.0
N3B—C4B—C5B	118.7 (2)	C3D—C4D—C5D	120.2 (2)
C6B—C5B—C4B	119.7 (2)	C3D—C4D—H4DA	119.9
C6B—C5B—Cl2	121.73 (19)	C5D—C4D—H4DA	119.9

C4B—C5B—Cl2	118.5 (2)	C6D—C5D—C4D	119.3 (3)
N1B—C6B—C5B	120.4 (2)	C6D—C5D—H5DA	120.4
N1B—C6B—C8B	116.5 (2)	C4D—C5D—H5DA	120.4
C5B—C6B—C8B	123.1 (2)	C5D—C6D—C1D	120.8 (2)
C2B—C7B—H7BA	109.5	C5D—C6D—H6DA	119.6
C2B—C7B—H7BB	109.5	C1D—C6D—H6DA	119.6
H7BA—C7B—H7BB	109.5	O2D—C7D—O1D	122.1 (2)
C2B—C7B—H7BC	109.5	O2D—C7D—C1D	124.7 (2)
H7BA—C7B—H7BC	109.5	O1D—C7D—C1D	113.2 (2)
H7BB—C7B—H7BC	109.5	C2D—C8D—H8DA	109.5
C6B—C8B—H8BA	109.5	C2D—C8D—H8DB	109.5
C6B—C8B—H8BB	109.5	H8DA—C8D—H8DB	109.5
H8BA—C8B—H8BB	109.5	C2D—C8D—H8DC	109.5
C6B—C8B—H8BC	109.5	H8DA—C8D—H8DC	109.5
H8BA—C8B—H8BC	109.5	H8DB—C8D—H8DC	109.5

C6A—N1A—C2A—N3A	−0.4 (4)	Cl2—C5B—C6B—C8B	−2.3 (4)
C6A—N1A—C2A—C7A	−179.8 (2)	C6C—C1C—C2C—C3C	0.5 (4)
N1A—C2A—N3A—C4A	−0.4 (4)	C7C—C1C—C2C—C3C	−177.4 (2)
C7A—C2A—N3A—C4A	179.0 (2)	C6C—C1C—C2C—C8C	−178.8 (3)
C2A—N3A—C4A—N4A	−178.4 (3)	C7C—C1C—C2C—C8C	3.4 (4)
C2A—N3A—C4A—C5A	1.7 (4)	C1C—C2C—C3C—C4C	0.9 (4)
N4A—C4A—C5A—C6A	177.9 (3)	C8C—C2C—C3C—C4C	−179.8 (3)
N3A—C4A—C5A—C6A	−2.2 (4)	C2C—C3C—C4C—C5C	−1.1 (4)
N4A—C4A—C5A—Cl1	−1.9 (4)	C3C—C4C—C5C—C6C	−0.1 (4)
N3A—C4A—C5A—Cl1	178.0 (2)	C4C—C5C—C6C—C1C	1.5 (4)
C2A—N1A—C6A—C5A	−0.1 (4)	C2C—C1C—C6C—C5C	−1.7 (4)
C2A—N1A—C6A—C8A	179.2 (2)	C7C—C1C—C6C—C5C	176.2 (3)
C4A—C5A—C6A—N1A	1.4 (4)	C6C—C1C—C7C—O2C	−159.6 (3)
Cl1—C5A—C6A—N1A	−178.8 (2)	C2C—C1C—C7C—O2C	18.3 (4)
C4A—C5A—C6A—C8A	−177.9 (2)	C6C—C1C—C7C—O1C	18.1 (4)
Cl1—C5A—C6A—C8A	1.9 (4)	C2C—C1C—C7C—O1C	−164.0 (3)
C6B—N1B—C2B—N3B	1.1 (4)	C6D—C1D—C2D—C3D	3.6 (4)
C6B—N1B—C2B—C7B	−179.2 (2)	C7D—C1D—C2D—C3D	−176.8 (2)
N1B—C2B—N3B—C4B	−1.2 (4)	C6D—C1D—C2D—C8D	−177.2 (3)
C7B—C2B—N3B—C4B	179.1 (2)	C7D—C1D—C2D—C8D	2.4 (4)
C2B—N3B—C4B—N4B	−180.0 (3)	C1D—C2D—C3D—C4D	−2.9 (4)
C2B—N3B—C4B—C5B	−0.3 (4)	C8D—C2D—C3D—C4D	177.8 (3)
N4B—C4B—C5B—C6B	−178.5 (3)	C2D—C3D—C4D—C5D	0.8 (4)
N3B—C4B—C5B—C6B	1.9 (4)	C3D—C4D—C5D—C6D	0.8 (4)
N4B—C4B—C5B—Cl2	1.3 (4)	C4D—C5D—C6D—C1D	−0.1 (4)
N3B—C4B—C5B—Cl2	−178.3 (2)	C2D—C1D—C6D—C5D	−2.2 (4)
C2B—N1B—C6B—C5B	0.5 (4)	C7D—C1D—C6D—C5D	178.2 (2)
C2B—N1B—C6B—C8B	−179.0 (2)	C6D—C1D—C7D—O2D	162.9 (3)
C4B—C5B—C6B—N1B	−2.0 (4)	C2D—C1D—C7D—O2D	−16.7 (4)
Cl2—C5B—C6B—N1B	178.2 (2)	C6D—C1D—C7D—O1D	−16.7 (4)
C4B—C5B—C6B—C8B	177.5 (2)	C2D—C1D—C7D—O1D	163.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4*A*—H4*AA*···O2*C*	0.88	2.07	2.938 (3)	169
N4*A*—H4*AB*···N1*B*	0.88	2.39	3.104 (3)	139
C7*A*—H7*AA*···Cl2^{i}	0.98	2.84	3.816 (3)	173
C7*A*—H7*AB*···O1*C*	0.98	2.54	3.281 (3)	132
N4*B*—H4*BA*···O2*D*	0.88	2.07	2.938 (3)	170
N4*B*—H4*BB*···N1*A*^{ii}	0.88	2.42	3.164 (3)	142
C7*B*—H7*BA*···Cl1	0.98	2.94	3.783 (3)	145
O1*C*—H1*C*···N3*A*	0.96 (5)	1.70 (5)	2.662 (3)	174 (5)
O1*D*—H1*D*···N3*B*	0.95 (4)	1.75 (4)	2.685 (3)	170 (4)

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

4-Amino-5-chloro-2,6-dimethylpyrimidine–3-methylbenzoic acid (1/1) (COCRYSTAL-8)

Crystal data

$C_6H_8ClN_3·C_8H_8O_2$
M_r = 293.75
Orthorhombic, *Pbcn*
a = 8.4524 (1) Å
b = 13.5387 (2) Å
c = 24.9813 (3) Å
V = 2858.72 (6) Å^3
Z = 8
F(000) = 1232
D_x = 1.365 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 15282 reflections
θ = 3.6–76.6°
μ = 2.42 mm^{-1}
T = 120 K
Prism, colorless
0.42 × 0.24 × 0.19 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: sealed X-ray tube
Detector resolution: 10.6501 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.680, T_{max} = 1.000
26401 measured reflections
3006 independent reflections
2904 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 76.8°, θ_{min} = 3.5°
h = −7→10
k = −15→16
l = −30→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.103
S = 1.04
3006 reflections
196 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 1.3483P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.15056 (4)	0.43229 (2)	0.19457 (2)	0.02742 (13)
N1A	0.27927 (13)	0.68415 (8)	0.26427 (4)	0.0221 (2)
C2A	0.35774 (15)	0.64739 (10)	0.30611 (5)	0.0203 (3)
N3A	0.38017 (13)	0.55115 (8)	0.31659 (4)	0.0201 (2)
N4A	0.33933 (14)	0.38852 (9)	0.29368 (5)	0.0238 (3)
H41	0.391 (2)	0.3742 (13)	0.3208 (7)	0.024 (4)*
H42	0.297 (2)	0.3408 (15)	0.2732 (8)	0.041 (5)*
C4A	0.31709 (15)	0.48386 (9)	0.28280 (5)	0.0196 (3)
C5A	0.23205 (15)	0.51817 (9)	0.23781 (5)	0.0208 (3)
C6A	0.21632 (15)	0.61794 (10)	0.22941 (5)	0.0218 (3)
C7A	0.42722 (17)	0.71901 (9)	0.34549 (5)	0.0272 (3)
H7AA	0.4024	0.7867	0.3343	0.041*
H7AB	0.5423	0.7104	0.3468	0.041*
H7AC	0.3824	0.7068	0.3810	0.041*
C8A	0.13053 (17)	0.65888 (11)	0.18186 (6)	0.0292 (3)
H8AA	0.1421	0.7309	0.1812	0.044*
H8AB	0.0181	0.6418	0.1843	0.044*
H8AC	0.1752	0.6308	0.1490	0.044*
O1B	0.56542 (12)	0.51547 (7)	0.40098 (4)	0.0260 (2)
H1B	0.502 (3)	0.5220 (17)	0.3730 (9)	0.056 (6)*
O2B	0.51805 (11)	0.35371 (7)	0.39001 (4)	0.0259 (2)
C1B	0.68785 (15)	0.40432 (10)	0.46069 (5)	0.0218 (3)
C2B	0.73386 (15)	0.48174 (10)	0.49402 (5)	0.0231 (3)
H2BA	0.6996	0.5470	0.4863	0.028*
C3B	0.82943 (16)	0.46448 (11)	0.53845 (5)	0.0254 (3)
C4B	0.87966 (17)	0.36796 (11)	0.54822 (6)	0.0296 (3)
H4BA	0.9452	0.3549	0.5783	0.035*
C5B	0.83573 (18)	0.29079 (11)	0.51486 (6)	0.0324 (3)
H5BA	0.8722	0.2257	0.5220	0.039*
C6B	0.73882 (17)	0.30830 (10)	0.47111 (6)	0.0277 (3)
H6BA	0.7075	0.2554	0.4485	0.033*
C7B	0.58274 (15)	0.42178 (9)	0.41389 (5)	0.0213 (3)
C8B	0.87751 (18)	0.54831 (12)	0.57482 (6)	0.0312 (3)
H8BA	0.9427	0.5226	0.6041	0.047*
H8BB	0.7827	0.5798	0.5896	0.047*
H8BC	0.9384	0.5970	0.5544	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0331 (2)	0.0262 (2)	0.02299 (19)	−0.00227 (12)	−0.00619 (12)	−0.00403 (11)
N1A	0.0231 (5)	0.0199 (5)	0.0233 (5)	0.0012 (4)	0.0003 (4)	0.0013 (4)
C2A	0.0201 (6)	0.0183 (6)	0.0225 (6)	−0.0007 (4)	0.0018 (4)	0.0009 (4)
N3A	0.0214 (5)	0.0187 (5)	0.0203 (5)	−0.0009 (4)	−0.0010 (4)	0.0003 (4)
N4A	0.0306 (6)	0.0184 (6)	0.0225 (6)	−0.0004 (4)	−0.0057 (5)	0.0001 (4)

C4A	0.0195 (5)	0.0194 (6)	0.0200 (6)	−0.0012 (5)	0.0031 (5)	−0.0003 (4)
C5A	0.0205 (6)	0.0227 (6)	0.0193 (6)	−0.0011 (5)	0.0001 (5)	−0.0018 (4)
C6A	0.0197 (6)	0.0252 (6)	0.0206 (6)	0.0016 (5)	0.0012 (5)	0.0012 (5)
C7A	0.0323 (7)	0.0204 (6)	0.0290 (7)	−0.0019 (5)	−0.0043 (5)	−0.0012 (5)
C8A	0.0313 (7)	0.0290 (7)	0.0271 (7)	0.0044 (6)	−0.0052 (6)	0.0044 (6)
O1B	0.0317 (5)	0.0204 (5)	0.0260 (5)	0.0007 (4)	−0.0091 (4)	0.0009 (4)
O2B	0.0292 (5)	0.0226 (5)	0.0259 (5)	−0.0029 (4)	−0.0062 (4)	0.0006 (3)
C1B	0.0189 (6)	0.0249 (6)	0.0217 (6)	−0.0010 (5)	−0.0001 (5)	0.0023 (5)
C2B	0.0208 (6)	0.0257 (7)	0.0229 (6)	0.0008 (5)	0.0005 (5)	−0.0003 (5)
C3B	0.0206 (6)	0.0336 (7)	0.0222 (6)	−0.0019 (5)	0.0005 (5)	−0.0006 (5)
C4B	0.0250 (6)	0.0359 (8)	0.0278 (7)	−0.0007 (6)	−0.0064 (5)	0.0060 (6)
C5B	0.0320 (7)	0.0262 (7)	0.0390 (8)	0.0002 (6)	−0.0101 (6)	0.0074 (6)
C6B	0.0265 (7)	0.0244 (7)	0.0323 (7)	−0.0022 (5)	−0.0059 (5)	0.0023 (5)
C7B	0.0198 (6)	0.0227 (6)	0.0214 (6)	0.0005 (5)	0.0013 (5)	0.0009 (5)
C8B	0.0287 (7)	0.0394 (8)	0.0254 (7)	−0.0002 (6)	−0.0042 (5)	−0.0063 (6)

Geometric parameters (Å, º)

Cl1—C5A	1.7301 (13)	O1B—C7B	1.3169 (16)
N1A—C2A	1.3342 (17)	O1B—H1B	0.88 (2)
N1A—C6A	1.3584 (17)	O2B—C7B	1.2264 (16)
C2A—N3A	1.3424 (17)	C1B—C6B	1.3940 (18)
C2A—C7A	1.5011 (18)	C1B—C2B	1.3940 (18)
N3A—C4A	1.3516 (16)	C1B—C7B	1.4874 (18)
N4A—C4A	1.3325 (17)	C2B—C3B	1.3924 (18)
N4A—H41	0.829 (18)	C2B—H2BA	0.9500
N4A—H42	0.90 (2)	C3B—C4B	1.396 (2)
C4A—C5A	1.4125 (18)	C3B—C8B	1.510 (2)
C5A—C6A	1.3735 (19)	C4B—C5B	1.387 (2)
C6A—C8A	1.4979 (18)	C4B—H4BA	0.9500
C7A—H7AA	0.9800	C5B—C6B	1.386 (2)
C7A—H7AB	0.9800	C5B—H5BA	0.9500
C7A—H7AC	0.9800	C6B—H6BA	0.9500
C8A—H8AA	0.9800	C8B—H8BA	0.9800
C8A—H8AB	0.9800	C8B—H8BB	0.9800
C8A—H8AC	0.9800	C8B—H8BC	0.9800
C2A—N1A—C6A	116.79 (11)	C7B—O1B—H1B	110.9 (15)
N1A—C2A—N3A	125.81 (12)	C6B—C1B—C2B	120.23 (12)
N1A—C2A—C7A	117.83 (12)	C6B—C1B—C7B	118.66 (12)
N3A—C2A—C7A	116.35 (11)	C2B—C1B—C7B	121.11 (12)
C2A—N3A—C4A	118.47 (11)	C3B—C2B—C1B	120.78 (13)
C4A—N4A—H41	117.9 (12)	C3B—C2B—H2BA	119.6
C4A—N4A—H42	121.6 (13)	C1B—C2B—H2BA	119.6
H41—N4A—H42	120.5 (18)	C2B—C3B—C4B	118.23 (13)
N4A—C4A—N3A	118.03 (12)	C2B—C3B—C8B	120.65 (14)
N4A—C4A—C5A	123.55 (12)	C4B—C3B—C8B	121.12 (13)
N3A—C4A—C5A	118.42 (11)	C5B—C4B—C3B	121.25 (13)

C6A—C5A—C4A	119.62 (11)	C5B—C4B—H4BA	119.4
C6A—C5A—Cl1	121.80 (10)	C3B—C4B—H4BA	119.4
C4A—C5A—Cl1	118.58 (10)	C6B—C5B—C4B	120.20 (14)
N1A—C6A—C5A	120.87 (11)	C6B—C5B—H5BA	119.9
N1A—C6A—C8A	116.99 (12)	C4B—C5B—H5BA	119.9
C5A—C6A—C8A	122.14 (12)	C5B—C6B—C1B	119.30 (13)
C2A—C7A—H7AA	109.5	C5B—C6B—H6BA	120.3
C2A—C7A—H7AB	109.5	C1B—C6B—H6BA	120.3
H7AA—C7A—H7AB	109.5	O2B—C7B—O1B	123.72 (12)
C2A—C7A—H7AC	109.5	O2B—C7B—C1B	121.95 (12)
H7AA—C7A—H7AC	109.5	O1B—C7B—C1B	114.33 (11)
H7AB—C7A—H7AC	109.5	C3B—C8B—H8BA	109.5
C6A—C8A—H8AA	109.5	C3B—C8B—H8BB	109.5
C6A—C8A—H8AB	109.5	H8BA—C8B—H8BB	109.5
H8AA—C8A—H8AB	109.5	C3B—C8B—H8BC	109.5
C6A—C8A—H8AC	109.5	H8BA—C8B—H8BC	109.5
H8AA—C8A—H8AC	109.5	H8BB—C8B—H8BC	109.5
H8AB—C8A—H8AC	109.5		

C6A—N1A—C2A—N3A	0.22 (19)	Cl1—C5A—C6A—C8A	−1.18 (18)
C6A—N1A—C2A—C7A	−179.47 (11)	C6B—C1B—C2B—C3B	−0.8 (2)
N1A—C2A—N3A—C4A	−0.97 (19)	C7B—C1B—C2B—C3B	178.57 (12)
C7A—C2A—N3A—C4A	178.73 (11)	C1B—C2B—C3B—C4B	0.9 (2)
C2A—N3A—C4A—N4A	−179.68 (12)	C1B—C2B—C3B—C8B	−179.30 (13)
C2A—N3A—C4A—C5A	0.64 (18)	C2B—C3B—C4B—C5B	−0.2 (2)
N4A—C4A—C5A—C6A	−179.33 (12)	C8B—C3B—C4B—C5B	−179.97 (14)
N3A—C4A—C5A—C6A	0.33 (18)	C3B—C4B—C5B—C6B	−0.7 (2)
N4A—C4A—C5A—Cl1	0.54 (18)	C4B—C5B—C6B—C1B	0.8 (2)
N3A—C4A—C5A—Cl1	−179.80 (9)	C2B—C1B—C6B—C5B	−0.1 (2)
C2A—N1A—C6A—C5A	0.82 (18)	C7B—C1B—C6B—C5B	−179.46 (13)
C2A—N1A—C6A—C8A	−178.96 (11)	C6B—C1B—C7B—O2B	12.8 (2)
C4A—C5A—C6A—N1A	−1.09 (19)	C2B—C1B—C7B—O2B	−166.53 (12)
Cl1—C5A—C6A—N1A	179.04 (10)	C6B—C1B—C7B—O1B	−167.53 (12)
C4A—C5A—C6A—C8A	178.68 (12)	C2B—C1B—C7B—O1B	13.12 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4*A*—H41···O2*B*	0.829 (18)	2.055 (19)	2.8802 (15)	174.2 (17)
N4*A*—H42···N1*A*^{i}	0.90 (2)	2.23 (2)	3.0332 (16)	149.0 (17)
C7*A*—H7*AA*···Cl1^{ii}	0.98	2.97	3.5919 (14)	123
C7*A*—H7*AA*···N4*A*^{iii}	0.98	2.67	3.4667 (18)	139
C8*A*—H8*AA*···O2*B*^{iv}	0.98	2.65	3.3295 (17)	127
O1*B*—H1*B*···N3*A*	0.88 (2)	1.79 (2)	2.6701 (15)	173 (2)

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

4-Amino-5-chloro-2,6-dimethylpyrimidine–4-methylbenzoic acid (1/1) (COCRYSTAL-9)

Crystal data

$C_6H_8ClN_3 \cdot C_8H_8O_2$
$M_r = 293.75$
Monoclinic, $P2_1/c$
$a = 8.0223$ (5) Å
$b = 13.6901$ (10) Å
$c = 13.3346$ (10) Å
$\beta = 101.557$ (7)°
$V = 1434.80$ (18) Å^3
$Z = 4$
$F(000) = 616$
$D_x = 1.360$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2368 reflections
$\theta = 4.7$–$76.5°$
$\mu = 2.41$ mm^{-1}
$T = 120$ K
Plate, colorless
0.51 × 0.17 × 0.08 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: sealed X-ray tube
Detector resolution: 10.6501 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
$T_{min} = 0.582$, $T_{max} = 1.000$
6765 measured reflections
2966 independent reflections
2422 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 76.7°$, $\theta_{min} = 4.7°$
$h = -8 \rightarrow 10$
$k = -17 \rightarrow 17$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.140$
$S = 1.04$
2966 reflections
197 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0813P)^2 + 0.4428P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0014 (4)

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	1.08463 (7)	0.85968 (4)	0.61237 (4)	0.03229 (19)
N1A	0.9592 (2)	0.72109 (13)	0.34491 (13)	0.0271 (4)
C2A	0.8839 (3)	0.64300 (15)	0.37583 (16)	0.0264 (4)
N3A	0.8637 (2)	0.62518 (13)	0.47148 (13)	0.0262 (4)
N4A	0.8970 (2)	0.67557 (14)	0.63951 (14)	0.0297 (4)
H41	0.852 (3)	0.625 (2)	0.647 (2)	0.030 (7)*
H42	0.934 (3)	0.719 (2)	0.691 (2)	0.042 (7)*
C4A	0.9222 (2)	0.69202 (15)	0.54527 (15)	0.0253 (4)

C5A	1.0068 (2)	0.77534 (15)	0.51821 (15)	0.0265 (4)
C6A	1.0238 (2)	0.78780 (15)	0.41779 (15)	0.0259 (4)
C7A	0.8182 (3)	0.56630 (16)	0.29745 (16)	0.0323 (5)
H7AA	0.8067	0.5941	0.2287	0.048*
H7AB	0.7069	0.5434	0.3073	0.048*
H7AC	0.8980	0.5113	0.3051	0.048*
C8A	1.1093 (3)	0.87516 (16)	0.38284 (17)	0.0308 (4)
H8AA	1.1603	0.8570	0.3246	0.046*
H8AB	1.1984	0.8986	0.4390	0.046*
H8AC	1.0252	0.9270	0.3621	0.046*
O1B	0.7077 (2)	0.45998 (12)	0.49384 (12)	0.0375 (4)
H1B	0.757 (5)	0.519 (3)	0.492 (3)	0.089 (13)*
O2B	0.7255 (2)	0.48776 (12)	0.66154 (12)	0.0373 (4)
C1B	0.5926 (3)	0.34164 (16)	0.58705 (17)	0.0288 (4)
C2B	0.5582 (3)	0.30639 (17)	0.67918 (17)	0.0310 (5)
H2BA	0.5902	0.3436	0.7401	0.037*
C3B	0.4773 (3)	0.21712 (17)	0.68174 (17)	0.0321 (5)
H3BA	0.4540	0.1940	0.7447	0.038*
C4B	0.4296 (3)	0.16065 (16)	0.59342 (17)	0.0304 (5)
C5B	0.4629 (3)	0.19749 (17)	0.50191 (17)	0.0328 (5)
H5BA	0.4295	0.1608	0.4407	0.039*
C6B	0.5437 (3)	0.28656 (16)	0.49835 (16)	0.0304 (5)
H6BA	0.5658	0.3100	0.4352	0.037*
C7B	0.6814 (3)	0.43686 (16)	0.58525 (16)	0.0298 (4)
C8B	0.3480 (3)	0.06233 (18)	0.59702 (19)	0.0384 (5)
H8BA	0.2421	0.0597	0.5456	0.058*
H8BB	0.3230	0.0518	0.6652	0.058*
H8BC	0.4258	0.0114	0.5826	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0424 (3)	0.0267 (3)	0.0290 (3)	−0.00801 (19)	0.0100 (2)	−0.00421 (18)
N1A	0.0310 (8)	0.0251 (9)	0.0267 (8)	−0.0005 (7)	0.0094 (6)	−0.0003 (7)
C2A	0.0289 (9)	0.0233 (10)	0.0279 (10)	0.0017 (7)	0.0083 (8)	−0.0017 (8)
N3A	0.0303 (8)	0.0220 (8)	0.0274 (8)	−0.0006 (7)	0.0080 (6)	0.0003 (7)
N4A	0.0422 (10)	0.0216 (9)	0.0263 (9)	−0.0077 (8)	0.0096 (7)	−0.0003 (7)
C4A	0.0281 (9)	0.0222 (9)	0.0262 (9)	0.0017 (7)	0.0068 (7)	0.0010 (8)
C5A	0.0282 (9)	0.0226 (10)	0.0298 (10)	0.0008 (8)	0.0081 (8)	−0.0012 (8)
C6A	0.0257 (9)	0.0225 (10)	0.0307 (10)	0.0021 (7)	0.0086 (7)	0.0019 (8)
C7A	0.0425 (11)	0.0280 (11)	0.0286 (10)	−0.0036 (9)	0.0124 (8)	−0.0041 (9)
C8A	0.0351 (10)	0.0279 (10)	0.0312 (10)	−0.0025 (9)	0.0112 (8)	0.0020 (8)
O1B	0.0513 (10)	0.0307 (8)	0.0339 (8)	−0.0130 (7)	0.0165 (7)	−0.0017 (7)
O2B	0.0485 (9)	0.0316 (8)	0.0331 (8)	−0.0099 (7)	0.0113 (7)	−0.0036 (7)
C1B	0.0282 (10)	0.0251 (10)	0.0340 (10)	−0.0005 (8)	0.0088 (8)	0.0000 (8)
C2B	0.0321 (10)	0.0306 (11)	0.0309 (10)	−0.0025 (9)	0.0076 (8)	−0.0012 (9)
C3B	0.0330 (10)	0.0334 (12)	0.0315 (10)	−0.0023 (9)	0.0105 (8)	0.0042 (9)
C4B	0.0272 (10)	0.0266 (10)	0.0383 (11)	0.0003 (8)	0.0091 (8)	0.0008 (9)

C5B	0.0359 (11)	0.0276 (11)	0.0352 (11)	−0.0023 (9)	0.0081 (9)	−0.0044 (9)
C6B	0.0341 (10)	0.0287 (11)	0.0295 (10)	−0.0016 (8)	0.0087 (8)	0.0009 (8)
C7B	0.0305 (10)	0.0274 (10)	0.0329 (10)	0.0000 (8)	0.0092 (8)	0.0005 (9)
C8B	0.0407 (12)	0.0297 (12)	0.0470 (13)	−0.0035 (9)	0.0138 (10)	0.0027 (10)

Geometric parameters (Å, º)

Cl1—C5A	1.728 (2)	O1B—C7B	1.317 (3)
N1A—C2A	1.333 (3)	O1B—H1B	0.90 (4)
N1A—C6A	1.358 (3)	O2B—C7B	1.225 (3)
C2A—N3A	1.340 (3)	C1B—C6B	1.391 (3)
C2A—C7A	1.501 (3)	C1B—C2B	1.398 (3)
N3A—C4A	1.357 (3)	C1B—C7B	1.488 (3)
N4A—C4A	1.331 (3)	C2B—C3B	1.387 (3)
N4A—H41	0.79 (3)	C2B—H2BA	0.9500
N4A—H42	0.91 (3)	C3B—C4B	1.397 (3)
C4A—C5A	1.410 (3)	C3B—H3BA	0.9500
C5A—C6A	1.383 (3)	C4B—C5B	1.395 (3)
C6A—C8A	1.499 (3)	C4B—C8B	1.502 (3)
C7A—H7AA	0.9800	C5B—C6B	1.386 (3)
C7A—H7AB	0.9800	C5B—H5BA	0.9500
C7A—H7AC	0.9800	C6B—H6BA	0.9500
C8A—H8AA	0.9800	C8B—H8BA	0.9800
C8A—H8AB	0.9800	C8B—H8BB	0.9800
C8A—H8AC	0.9800	C8B—H8BC	0.9800
C2A—N1A—C6A	116.70 (17)	C7B—O1B—H1B	113 (3)
N1A—C2A—N3A	126.09 (19)	C6B—C1B—C2B	119.2 (2)
N1A—C2A—C7A	117.61 (18)	C6B—C1B—C7B	121.0 (2)
N3A—C2A—C7A	116.28 (18)	C2B—C1B—C7B	119.7 (2)
C2A—N3A—C4A	118.50 (18)	C3B—C2B—C1B	120.1 (2)
C4A—N4A—H41	114.9 (19)	C3B—C2B—H2BA	120.0
C4A—N4A—H42	121.2 (18)	C1B—C2B—H2BA	120.0
H41—N4A—H42	124 (3)	C2B—C3B—C4B	121.2 (2)
N4A—C4A—N3A	118.32 (19)	C2B—C3B—H3BA	119.4
N4A—C4A—C5A	123.37 (19)	C4B—C3B—H3BA	119.4
N3A—C4A—C5A	118.31 (18)	C5B—C4B—C3B	118.0 (2)
C6A—C5A—C4A	119.55 (19)	C5B—C4B—C8B	120.9 (2)
C6A—C5A—Cl1	121.97 (16)	C3B—C4B—C8B	121.1 (2)
C4A—C5A—Cl1	118.48 (15)	C6B—C5B—C4B	121.4 (2)
N1A—C6A—C5A	120.80 (18)	C6B—C5B—H5BA	119.3
N1A—C6A—C8A	116.54 (18)	C4B—C5B—H5BA	119.3
C5A—C6A—C8A	122.64 (19)	C5B—C6B—C1B	120.1 (2)
C2A—C7A—H7AA	109.5	C5B—C6B—H6BA	119.9
C2A—C7A—H7AB	109.5	C1B—C6B—H6BA	119.9
H7AA—C7A—H7AB	109.5	O2B—C7B—O1B	124.0 (2)
C2A—C7A—H7AC	109.5	O2B—C7B—C1B	123.0 (2)
H7AA—C7A—H7AC	109.5	O1B—C7B—C1B	113.06 (19)

H7AB—C7A—H7AC	109.5	C4B—C8B—H8BA	109.5
C6A—C8A—H8AA	109.5	C4B—C8B—H8BB	109.5
C6A—C8A—H8AB	109.5	H8BA—C8B—H8BB	109.5
H8AA—C8A—H8AB	109.5	C4B—C8B—H8BC	109.5
C6A—C8A—H8AC	109.5	H8BA—C8B—H8BC	109.5
H8AA—C8A—H8AC	109.5	H8BB—C8B—H8BC	109.5
H8AB—C8A—H8AC	109.5		

C6A—N1A—C2A—N3A	1.2 (3)	Cl1—C5A—C6A—C8A	−0.5 (3)
C6A—N1A—C2A—C7A	−177.48 (18)	C6B—C1B—C2B—C3B	0.5 (3)
N1A—C2A—N3A—C4A	0.8 (3)	C7B—C1B—C2B—C3B	−179.18 (19)
C7A—C2A—N3A—C4A	179.52 (18)	C1B—C2B—C3B—C4B	0.3 (3)
C2A—N3A—C4A—N4A	177.86 (18)	C2B—C3B—C4B—C5B	−1.1 (3)
C2A—N3A—C4A—C5A	−2.2 (3)	C2B—C3B—C4B—C8B	177.7 (2)
N4A—C4A—C5A—C6A	−178.43 (19)	C3B—C4B—C5B—C6B	1.2 (3)
N3A—C4A—C5A—C6A	1.6 (3)	C8B—C4B—C5B—C6B	−177.6 (2)
N4A—C4A—C5A—Cl1	1.0 (3)	C4B—C5B—C6B—C1B	−0.4 (3)
N3A—C4A—C5A—Cl1	−178.94 (14)	C2B—C1B—C6B—C5B	−0.4 (3)
C2A—N1A—C6A—C5A	−1.8 (3)	C7B—C1B—C6B—C5B	179.21 (19)
C2A—N1A—C6A—C8A	179.60 (17)	C6B—C1B—C7B—O2B	179.5 (2)
C4A—C5A—C6A—N1A	0.4 (3)	C2B—C1B—C7B—O2B	−0.8 (3)
Cl1—C5A—C6A—N1A	−179.01 (15)	C6B—C1B—C7B—O1B	−0.7 (3)
C4A—C5A—C6A—C8A	178.96 (18)	C2B—C1B—C7B—O1B	178.94 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4*A*—H41···O2*B*	0.79 (3)	2.17 (3)	2.958 (2)	178 (3)
N4*A*—H42···N1*A*^{i}	0.91 (3)	2.18 (3)	3.034 (2)	156 (2)
O1*B*—H1*B*···N3*A*	0.90 (4)	1.74 (4)	2.630 (2)	171 (4)

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

4-Amino-5-chloro-2,6-dimethylpyrimidine–4-aminobenzoic acid (1/1) (COCRYSTAL-10)

Crystal data

$C_6H_8ClN_3·C_7H_7NO_2$
M_r = 294.74
Monoclinic, $P2_1/c$
a = 7.8899 (2) Å
b = 13.2361 (3) Å
c = 13.3212 (3) Å
β = 101.254 (2)°
V = 1364.40 (6) Å^3
Z = 4
$F(000)$ = 616
D_x = 1.435 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 4256 reflections
θ = 3.3–76.1°
μ = 2.56 mm^{-1}
T = 120 K
Chunk, colorless
0.41 × 0.35 × 0.24 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: sealed X-ray tube
Detector resolution: 10.6501 pixels mm^{-1}
ω scans

Absorption correction: multi-scan
(CrysAlis PRO; Agilent, 2014)
T_{min} = 0.828, T_{max} = 1.000
6214 measured reflections
2823 independent reflections
2749 reflections with $I > 2\sigma(I)$

R_{int} = 0.017
θ_{max} = 76.7°, θ_{min} = 4.8°
h = −9→9
k = −16→15
l = −14→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
S = 1.04
2823 reflections
203 parameters
0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.5634P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	1.05069 (4)	0.86469 (2)	0.60646 (2)	0.02693 (12)
N1A	0.93400 (14)	0.71297 (8)	0.34395 (8)	0.0197 (2)
C2A	0.86103 (17)	0.63206 (10)	0.37710 (10)	0.0193 (3)
N3A	0.84090 (14)	0.61587 (8)	0.47345 (8)	0.0185 (2)
N4A	0.86802 (16)	0.67391 (9)	0.63872 (9)	0.0230 (3)
H4A1	0.817 (2)	0.6176 (15)	0.6497 (14)	0.028 (4)*
H4A2	0.897 (3)	0.7162 (16)	0.6858 (16)	0.037 (5)*
C4A	0.89549 (16)	0.68774 (10)	0.54425 (10)	0.0184 (3)
C5A	0.97806 (16)	0.77421 (9)	0.51419 (10)	0.0187 (3)
C6A	0.99586 (16)	0.78486 (10)	0.41444 (10)	0.0184 (3)
C7A	0.7941 (2)	0.55104 (11)	0.30121 (11)	0.0265 (3)
H7AA	0.8015	0.5740	0.2322	0.040*
H7AB	0.6734	0.5364	0.3040	0.040*
H7AC	0.8637	0.4898	0.3177	0.040*
C8A	1.07803 (18)	0.87473 (10)	0.37573 (11)	0.0226 (3)
H8AA	1.1481	0.8527	0.3266	0.034*
H8AB	1.1519	0.9092	0.4332	0.034*
H8AC	0.9880	0.9212	0.3420	0.034*
O1B	0.70377 (14)	0.43906 (8)	0.50497 (8)	0.0281 (2)
H1B	0.748 (3)	0.501 (2)	0.5011 (19)	0.052 (6)*
O2B	0.71164 (14)	0.47720 (7)	0.66954 (8)	0.0260 (2)
N1B	0.37076 (18)	0.03549 (10)	0.62891 (11)	0.0289 (3)
H1B1	0.352 (3)	0.0138 (16)	0.6885 (17)	0.035 (5)*
H1B2	0.329 (3)	0.0044 (17)	0.5724 (18)	0.041 (5)*

C1B	0.59620 (17)	0.31826 (10)	0.60438 (10)	0.0201 (3)
C2B	0.57168 (17)	0.28210 (10)	0.69932 (10)	0.0222 (3)
H2BA	0.6064	0.3224	0.7588	0.027*
C3B	0.49760 (18)	0.18860 (11)	0.70760 (10)	0.0232 (3)
H3BA	0.4834	0.1649	0.7728	0.028*
C4B	0.44307 (17)	0.12835 (10)	0.62039 (11)	0.0208 (3)
C5B	0.46641 (18)	0.16502 (10)	0.52511 (10)	0.0224 (3)
H5BA	0.4293	0.1257	0.4652	0.027*
C6B	0.54303 (17)	0.25799 (11)	0.51799 (10)	0.0225 (3)
H6BA	0.5598	0.2813	0.4532	0.027*
C7B	0.67560 (17)	0.41846 (10)	0.59684 (10)	0.0211 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0366 (2)	0.02105 (19)	0.02460 (19)	−0.01009 (12)	0.00947 (14)	−0.00687 (11)
N1A	0.0223 (5)	0.0179 (5)	0.0195 (5)	−0.0010 (4)	0.0059 (4)	−0.0004 (4)
C2A	0.0207 (6)	0.0180 (6)	0.0198 (6)	0.0001 (5)	0.0055 (5)	−0.0016 (5)
N3A	0.0217 (5)	0.0154 (5)	0.0191 (5)	−0.0017 (4)	0.0055 (4)	−0.0010 (4)
N4A	0.0335 (6)	0.0181 (6)	0.0181 (6)	−0.0068 (5)	0.0070 (5)	−0.0015 (4)
C4A	0.0194 (6)	0.0160 (6)	0.0197 (6)	0.0016 (4)	0.0037 (5)	−0.0001 (5)
C5A	0.0201 (6)	0.0154 (6)	0.0207 (6)	−0.0007 (5)	0.0046 (5)	−0.0015 (5)
C6A	0.0165 (5)	0.0163 (6)	0.0225 (6)	0.0015 (4)	0.0042 (5)	0.0010 (5)
C7A	0.0356 (7)	0.0226 (7)	0.0228 (7)	−0.0065 (6)	0.0095 (5)	−0.0056 (5)
C8A	0.0256 (6)	0.0189 (6)	0.0243 (7)	−0.0025 (5)	0.0074 (5)	0.0023 (5)
O1B	0.0412 (6)	0.0209 (5)	0.0248 (5)	−0.0089 (4)	0.0130 (4)	−0.0005 (4)
O2B	0.0358 (5)	0.0186 (5)	0.0255 (5)	−0.0047 (4)	0.0104 (4)	−0.0020 (4)
N1B	0.0371 (7)	0.0233 (6)	0.0274 (7)	−0.0114 (5)	0.0093 (5)	−0.0017 (5)
C1B	0.0200 (6)	0.0171 (6)	0.0241 (6)	−0.0002 (5)	0.0064 (5)	0.0006 (5)
C2B	0.0248 (6)	0.0205 (6)	0.0221 (6)	−0.0012 (5)	0.0064 (5)	−0.0015 (5)
C3B	0.0265 (7)	0.0225 (6)	0.0221 (6)	−0.0024 (5)	0.0088 (5)	0.0006 (5)
C4B	0.0177 (6)	0.0191 (6)	0.0263 (7)	−0.0008 (5)	0.0062 (5)	0.0006 (5)
C5B	0.0242 (6)	0.0211 (6)	0.0215 (6)	−0.0023 (5)	0.0034 (5)	−0.0028 (5)
C6B	0.0250 (6)	0.0222 (6)	0.0210 (6)	−0.0002 (5)	0.0062 (5)	0.0020 (5)
C7B	0.0225 (6)	0.0185 (6)	0.0234 (6)	0.0012 (5)	0.0069 (5)	0.0014 (5)

Geometric parameters (Å, º)

Cl1—C5A	1.7316 (13)	O1B—C7B	1.3145 (17)
N1A—C2A	1.3314 (17)	O1B—H1B	0.90 (3)
N1A—C6A	1.3589 (17)	O2B—C7B	1.2311 (17)
C2A—N3A	1.3410 (17)	N1B—C4B	1.3691 (17)
C2A—C7A	1.4975 (18)	N1B—H1B1	0.89 (2)
N3A—C4A	1.3497 (17)	N1B—H1B2	0.86 (2)
N4A—C4A	1.3307 (17)	C1B—C6B	1.3958 (19)
N4A—H4A1	0.87 (2)	C1B—C2B	1.4005 (19)
N4A—H4A2	0.84 (2)	C1B—C7B	1.4785 (18)
C4A—C5A	1.4129 (18)	C2B—C3B	1.3823 (19)

C5A—C6A	1.3704 (18)	C2B—H2BA	0.9500
C6A—C8A	1.4939 (17)	C3B—C4B	1.4056 (19)
C7A—H7AA	0.9800	C3B—H3BA	0.9500
C7A—H7AB	0.9800	C4B—C5B	1.4041 (19)
C7A—H7AC	0.9800	C5B—C6B	1.3824 (19)
C8A—H8AA	0.9800	C5B—H5BA	0.9500
C8A—H8AB	0.9800	C6B—H6BA	0.9500
C8A—H8AC	0.9800		

C2A—N1A—C6A	117.02 (11)	H8AA—C8A—H8AC	109.5
N1A—C2A—N3A	125.85 (12)	H8AB—C8A—H8AC	109.5
N1A—C2A—C7A	118.06 (12)	C7B—O1B—H1B	112.3 (16)
N3A—C2A—C7A	116.08 (11)	C4B—N1B—H1B1	120.9 (13)
C2A—N3A—C4A	118.35 (11)	C4B—N1B—H1B2	116.6 (14)
C4A—N4A—H4A1	116.2 (13)	H1B1—N1B—H1B2	122 (2)
C4A—N4A—H4A2	123.1 (14)	C6B—C1B—C2B	118.49 (12)
H4A1—N4A—H4A2	120.7 (19)	C6B—C1B—C7B	121.32 (12)
N4A—C4A—N3A	118.37 (12)	C2B—C1B—C7B	120.19 (12)
N4A—C4A—C5A	123.28 (12)	C3B—C2B—C1B	120.87 (13)
N3A—C4A—C5A	118.35 (11)	C3B—C2B—H2BA	119.6
C6A—C5A—C4A	119.89 (12)	C1B—C2B—H2BA	119.6
C6A—C5A—Cl1	122.33 (10)	C2B—C3B—C4B	120.53 (13)
C4A—C5A—Cl1	117.77 (10)	C2B—C3B—H3BA	119.7
N1A—C6A—C5A	120.47 (12)	C4B—C3B—H3BA	119.7
N1A—C6A—C8A	116.14 (11)	N1B—C4B—C5B	121.03 (13)
C5A—C6A—C8A	123.37 (12)	N1B—C4B—C3B	120.40 (13)
C2A—C7A—H7AA	109.5	C5B—C4B—C3B	118.56 (12)
C2A—C7A—H7AB	109.5	C6B—C5B—C4B	120.40 (12)
H7AA—C7A—H7AB	109.5	C6B—C5B—H5BA	119.8
C2A—C7A—H7AC	109.5	C4B—C5B—H5BA	119.8
H7AA—C7A—H7AC	109.5	C5B—C6B—C1B	121.15 (12)
H7AB—C7A—H7AC	109.5	C5B—C6B—H6BA	119.4
C6A—C8A—H8AA	109.5	C1B—C6B—H6BA	119.4
C6A—C8A—H8AB	109.5	O2B—C7B—O1B	123.12 (12)
H8AA—C8A—H8AB	109.5	O2B—C7B—C1B	123.29 (12)
C6A—C8A—H8AC	109.5	O1B—C7B—C1B	113.59 (12)

C6A—N1A—C2A—N3A	1.0 (2)	Cl1—C5A—C6A—C8A	−0.28 (18)
C6A—N1A—C2A—C7A	−179.14 (12)	C6B—C1B—C2B—C3B	0.4 (2)
N1A—C2A—N3A—C4A	1.3 (2)	C7B—C1B—C2B—C3B	179.99 (12)
C7A—C2A—N3A—C4A	−178.49 (12)	C1B—C2B—C3B—C4B	−0.9 (2)
C2A—N3A—C4A—N4A	176.81 (12)	C2B—C3B—C4B—N1B	179.58 (13)
C2A—N3A—C4A—C5A	−2.83 (18)	C2B—C3B—C4B—C5B	0.3 (2)
N4A—C4A—C5A—C6A	−177.52 (12)	N1B—C4B—C5B—C6B	−178.59 (13)
N3A—C4A—C5A—C6A	2.10 (19)	C3B—C4B—C5B—C6B	0.6 (2)
N4A—C4A—C5A—Cl1	1.49 (18)	C4B—C5B—C6B—C1B	−1.1 (2)
N3A—C4A—C5A—Cl1	−178.90 (9)	C2B—C1B—C6B—C5B	0.6 (2)
C2A—N1A—C6A—C5A	−1.78 (18)	C7B—C1B—C6B—C5B	−178.99 (12)

C2A—N1A—C6A—C8A	179.69 (11)	C6B—C1B—C7B—O2B	174.06 (13)
C4A—C5A—C6A—N1A	0.26 (19)	C2B—C1B—C7B—O2B	−5.5 (2)
Cl1—C5A—C6A—N1A	−178.69 (9)	C6B—C1B—C7B—O1B	−5.78 (19)
C4A—C5A—C6A—C8A	178.68 (12)	C2B—C1B—C7B—O1B	174.67 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4*A*—H4*A*1···O2*B*	0.87 (2)	2.07 (2)	2.9441 (15)	174.7 (18)
N4*A*—H4*A*2···N1*A*^{i}	0.84 (2)	2.27 (2)	3.0710 (16)	159.5 (19)
C7*A*—H7*AA*···Cl1^{ii}	0.98	2.94	3.7580 (15)	142
C8*A*—H8*AC*···Cl1^{iii}	0.98	2.95	3.6163 (14)	127
O1*B*—H1*B*···N3*A*	0.90 (3)	1.76 (3)	2.6459 (15)	170 (2)
N1*B*—H1*B*1···O2*B*^{iv}	0.89 (2)	2.10 (2)	2.9847 (17)	173.4 (19)

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