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2-Amino-4,6-bis(4-chlorophenylthio)pyrimidine

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Key indicators

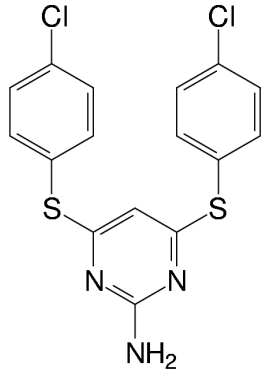
Single-crystal X-ray study
T = 151 K
Mean σ(C–C) = 0.004 Å
R factor = 0.056
wR factor = 0.148
Data-to-parameter ratio = 17.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The structure of the title compound, $C_{32}H_{22}Cl_4N_6S_4$, (I), comprises two unique molecules that separately associate *via* a three-centre N—H···N/S interaction to form two linear one-dimensional hydrogen-bonded chains. The dihedral angles between the two phenyl rings and the pyrimidine ring for each molecule are 84.6 (1) and 87.8 (1)°, and 83.9 (1) and 80.1 (1)°.

Experimental

Crystals of (I) were obtained from Spa Contract Synthesis.



(I)

Crystal data

$C_{32}H_{22}Cl_4N_6S_4$
M_r = 760.60
Monoclinic, $P2_1/c$
a = 28.4777 (13) Å
b = 8.6020 (3) Å
c = 14.2055 (5) Å
β = 102.5620 (13)°
V = 3396.5 (2) Å^3
Z = 4
D_x = 1.487 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12187 reflections
θ = 1.0–30.5°
μ = 0.63 mm^{-1}
T = 150 (2) K
Prism, colourless
0.15 × 0.15 × 0.10 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.912, T_{max} = 0.940
20 121 measured reflections
7363 independent reflections
4286 reflections with $I > 2\sigma(I)$
R_{int} = 0.080
θ_{max} = 27.5°
$h = -36 \rightarrow 37$
$k = -11 \rightarrow 10$
$l = -18 \rightarrow 17$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.148
S = 0.97
7363 reflections
432 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0703P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0046 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N21A—H21A···N3A^{i}	0.79 (4)	2.38 (4)	3.165 (4)	175 (3)
N21A—H21A···S7A^{i}	0.79 (4)	2.84 (3)	3.284 (3)	118 (3)
N21B—H21B···N3B^{ii}	0.82 (3)	2.37 (3)	3.187 (4)	178 (3)
N21B—H21B···S7B^{ii}	0.82 (3)	2.86 (3)	3.340 (3)	120 (2)

Symmetry codes: (i) $1-x, \frac{1}{2}+y, \frac{3}{2}-z$; (ii) $-x, \frac{1}{2}+y, \frac{1}{2}-z$.

All H atoms were included in the refinement, at calculated positions, as riding models with C—H set to 0.95 Å (Ar–H), except for the amine H atoms which were located on difference syntheses and both positional and displacement parameters refined.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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