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2-Amino-4-(4-chlorophenyl)-5,6-dihydrobenzo[*h*]quinoline-3-carbonitrile–3-amino-1-(4-chlorophenyl)-9,10-dihydrophenanthrene-2,4-dicarbonitrile (1/4)

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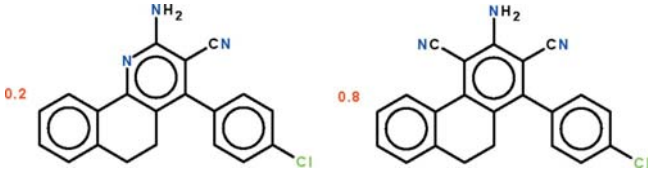
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.051; wR factor = 0.130; data-to-parameter ratio = 14.2.

The asymmetric unit of the 1:4 title co-crystal of 2-amino-4-(4-chlorophenyl)-5,6-dihydrobenzo[*h*]quinoline-3-carbonitrile and 3-amino-1-(4-chlorophenyl)-9,10-dihydrophenanthrene-2,4-dicarbonitrile, $0.2C_{20}H_{14}ClN_3\cdot0.8C_{22}H_{14}ClN_3$, has the atoms of the fused-ring system and those of the amino, cyano and chlorophenyl substitutents overlapped. The fused-ring system is buckled owing to the ethylene linkage in the central ring. There are two independent overlapped molecules in the asymmetric unit. In one independent molecule, the two flanking aromatic rings are twisted by 24.4 (1)° and the ring of the chlorophenyl substituent is twisted by 87.3 (1)° relative to the amino- and cyano-bearing aromatic ring. In the second molecule, the respective dihedral angles are 26.1 (1) and 57.8 (1)°. The two independent molecules are linked by N—H···N hydrogen bonds into dimers.

Related literature

For similar co-crystals, see: Asiri *et al.* (2011*a*,*b*).



Experimental

Crystal data

$0.2C_{20}H_{14}ClN_3\cdot0.8C_{22}H_{14}ClN_3$
M_r = 351.01
Monoclinic, $P2_1/c$
a = 19.2576 (7) Å
b = 9.5103 (2) Å
c = 20.2266 (7) Å
β = 114.018 (4)°
V = 3383.7 (2) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 2.06 mm^{-1}
T = 100 K
0.30 × 0.20 × 0.10 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.577, T_{max} = 0.821
12442 measured reflections
6686 independent reflections
6272 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.130
S = 1.05
6686 reflections
471 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21···N4	0.88	2.14	2.931 (3)	149
N5—H52···N3	0.88	2.33	3.136 (3)	152

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2147).

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