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2-Chloro-3-(pyrrolidin-1-yl)-1,4-naphthoquinone

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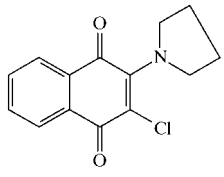
The structure of the title compound, $C_{14}H_{12}ClNO_2$, (I), comprises essentially planar molecules which crystallize in a monoclinic lattice. C—H···O interactions exist to both naphthoquinone O atoms and the Cl atom.



(I)

Experimental

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

Crystal data

$C_{14}H_{12}ClNO_2$
M_r = 261.70
Monoclinic, $P2_1/c$
a = 11.2926 (6) Å
b = 10.4429 (4) Å
c = 11.2028 (4) Å
β = 115.829 (15)°
V = 1189.14 (9) Å^3
Z = 4
D_x = 1.462 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6683 reflections
θ = 2.91–27.48°
μ = 0.313 mm^{-1}
T = 150 (2) K
Prism, red
0.20 × 0.17 × 0.10 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.940, T_{max} = 0.969
18 192 measured reflections
2729 independent reflections
1779 reflections with $I > 2\sigma(I)$
R_{int} = 0.109
θ_{max} = 27.51°
$h = -14 \rightarrow 14$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 14$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.118
S = 0.972
2729 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0635P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O4^{i}	0.95	2.53	3.281 (2)	136
C7—H7···O1^{ii}	0.95	2.41	3.254 (2)	149
C35—H351···O4^{iii}	0.99	2.53	3.398 (2)	146
C35—H352···Cl2	0.99	2.60	2.961 (2)	101

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

All H atoms were included in the refinement, at calculated positions, as riding models with C—H set to 0.95 (Ar–H) and 0.99 Å (CH_2).

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 (Sheldrick, 1997).

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