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Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.

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 H1C H 0.1309 0.2553 0.2395 0.049 Uiso 1 1 calc R . .
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 C5 C 0.2104(3) 0.5987(2) 0.6571(3) 0.0291(6) Uani 1 1 d . . .
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 C7 C 0.0452(2) 0.2450(2) 0.5609(2) 0.0241(5) Uani 1 1 d . . .
 C8 C -0.0039(3) 0.1394(3) 0.6165(3) 0.0374(7) Uani 1 1 d . . .
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 H8B H -0.0647 0.1578 0.6625 0.056 Uiso 1 1 calc R . .
 H8C H 0.0697 0.1303 0.6677 0.056 Uiso 1 1 calc R . .
 C9 C 0.0338(2) 0.2238(2) 0.4410(2) 0.0245(5) Uani 1 1 d . . .
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 C10 C 0.0379(2) 0.4017(2) 0.8213(2) 0.0241(5) Uani 1 1 d . . .
 H10 H -0.0470 0.4035 0.7940 0.029 Uiso 1 1 calc R . .
 C11 C 0.0956(2) 0.4114(2) 0.9325(2) 0.0215(5) Uani 1 1 d . . .
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 C12 C 0.2392(2) 0.3888(2) 0.8209(2) 0.0180(5) Uani 1 1 d . . .
 C13 C 0.3160(2) 0.4144(2) 1.0325(2) 0.0198(5) Uani 1 1 d . . .
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 C14 C 0.3896(3) 0.2470(2) 1.0983(2) 0.0239(5) Uani 1 1 d . . .
 H14 H 0.3698 0.2580 1.1729 0.029 Uiso 1 1 calc R . .
 C15 C 0.4436(3) 0.1654(2) 1.0512(2) 0.0249(5) Uani 1 1 d . . .
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 C16 C 0.4104(2) 0.2749(2) 0.9184(2) 0.0181(5) Uani 1 1 d . . .
 C17 C 0.5118(2) 0.1143(2) 0.8639(2) 0.0192(5) Uani 1 1 d . . .
 C18 C 0.6471(2) 0.1494(2) 0.8843(2) 0.0215(5) Uani 1 1 d . . .
 C19 C 0.7343(3) 0.2581(3) 0.9835(3) 0.0347(7) Uani 1 1 d . . .

H19A H 0.8253 0.2696 0.9819 0.052 Uiso 1 1 calc R . .
H19B H 0.7191 0.2415 1.0580 0.052 Uiso 1 1 calc R . .
H19C H 0.7150 0.3339 0.9751 0.052 Uiso 1 1 calc R . .
C20 C 0.6993(3) 0.0816(2) 0.8094(2) 0.0255(5) Uani 1 1 d . . .
H20 H 0.7911 0.1045 0.8219 0.031 Uiso 1 1 calc R . .
C21 C 0.6224(3) -0.0188(2) 0.7165(2) 0.0257(5) Uani 1 1 d . . .
C22 C 0.6817(3) -0.0929(3) 0.6379(3) 0.0379(7) Uani 1 1 d . . .
H22A H 0.6817 -0.0654 0.5656 0.057 Uiso 1 1 calc R . .
H22B H 0.6308 -0.1818 0.6191 0.057 Uiso 1 1 calc R . .
H22C H 0.7713 -0.0796 0.6778 0.057 Uiso 1 1 calc R . .
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H23 H 0.4339 -0.1176 0.6349 0.031 Uiso 1 1 calc R . .
C24 C 0.4307(2) 0.0155(2) 0.7707(2) 0.0241(5) Uani 1 1 d . . .
C25 C 0.2846(3) -0.0199(3) 0.7498(3) 0.0430(8) Uani 1 1 d . . .
H25A H 0.2578 -0.0345 0.8211 0.064 Uiso 1 1 calc R . .
H25B H 0.2437 -0.0961 0.6861 0.064 Uiso 1 1 calc R . .
H25C H 0.2576 0.0479 0.7285 0.064 Uiso 1 1 calc R . .
C26 C 0.4237(2) 0.3701(2) 0.6115(2) 0.0194(5) Uani 1 1 d . . .
H26 H 0.350(3) 0.337(2) 0.544(2) 0.013(6) Uiso 1 1 d . . .
C27 C 0.5075(2) 0.3059(2) 0.6561(2) 0.0206(5) Uani 1 1 d . . .
H27 H 0.498(3) 0.224(3) 0.627(3) 0.029(8) Uiso 1 1 d . . .
C28 C 0.6349(2) 0.3979(2) 0.7056(2) 0.0231(5) Uani 1 1 d . . .
C29 C 0.5029(2) 0.5004(2) 0.6351(2) 0.0204(5) Uani 1 1 d . . .
Cl1 Cl 0.05163(11) 0.08932(13) -0.06557(13) 0.0795(4) Uani 1 1 d . . .
C30 C 0.0833(7) 0.0023(7) 0.0184(8) 0.0520(19) Uani 0.50 1 d P . .
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 are estimated using the full covariance matrix. The cell esds are taken
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