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F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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O1 C2 C3 C4 -0.7(5).....?
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C31 O3 C3 C4 71.2(4).....?
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C71 O7 C7 C6 -6.2(5).....?
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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based
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on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ 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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H712 H 0.3606 0.3353 0.1908 0.070 Uiso 1 1 d ...
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 are estimated using the full covariance matrix. The cell esds are taken
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 used when they are defined by crystal symmetry. An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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O5 C5 1.358(2) .?
O5 H5 0.91(3) .?
O7 C7 1.370(2) .?
O7 C71 1.437(3) .?
O13 C13 1.365(2) .?
O13 H13 0.8505(13) .?
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O14 C141 1.431(2) .?
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C2 C11 1.473(2) .?
C3 C4 1.448(3) .?
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C4A C5 1.416(3).?
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C6 C7 1.392(3).?
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C7 C8 1.383(3).?
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C12 C13 1.374(2).?
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