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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 on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ 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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_geom_special_details

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only 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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 O9 Mn1 Mn2 38.2(12) . 1_655 ?
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 O8 Mn1 Mn2 83.0(12) . 2_666 ?
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 O6 Mn2 Mn2 133.1(13) 2_666 2_566 ?
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 O8 Mn2 Mn2 85.7(14) . 2_666 ?
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 O5 Mn2 Mn2 87.8(12) 2_666 2_666 ?
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