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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^ > 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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 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)
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Si O Ca 123.94(5) 2 58_566 ?
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Al O Ca 95.80(4) 28_445 58_566 ?
V O Ca 95.80(4) 28_445 58_566 ?
Ca O Ca 98.61(4) 49_556 58_566 ?
Mn O Ca 98.61(4) 49_556 58_566 ?
Mn O Ca 0.0 58_566 58_566 ?

_diffrn_measured_fraction_theta_max   0.979
_diffrn_reflns_theta_full   34.95
_diffrn_measured_fraction_theta_full   0.979
_refine_diff_density_max   0.351
_refine_diff_density_min   -0.347
_refine_diff_density_rms   0.088