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 'Al' 'Al' 0.0645 0.0514
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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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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0100P)^2^+0.8000P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
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_refine_ls_extinction_method   SHELXL
_refine_ls_extinction_coef   0.046(8)
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 'Flack H D (1983), Acta Cryst. A39, 876-881'
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 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)
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K O2 2.984(13) 2_544 ?
K O2 2.984(13) 1_454 ?
K O2 2.984(13) 4_664 ?
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