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'Al2 K1.97 O8 Si2'
_chemical_formula_weight 315.17

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_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
'O' 'O' 0.0106 0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Al' 'Al' 0.0645 0.0514
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Si' 'Si' 0.0817 0.0704
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'K' 'K' 0.2009 0.2494
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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'y, x, z+1/2'
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'-x, -x+y, z+1/2'
'x-y, -y, z+1/2'

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_cell_length_c 8.605(4)
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_diffn_reflns_limit_l_min       -14
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_reflns_threshold_expression     >2sigma(I)

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_computing_cell_refinement      ?
_computing_data_reduction       ?

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_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
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_computing_publication_material ?

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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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_refine_ls_weighting_details
'calc w=1/[sigma2(Fo2)+(0.0100P)2+0.8000P] where P=(Fo2+2Fc2)/3'
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_atom_sites_solution_secondary  difmap
_atom_sites_solution_hydrogens  geom
_refine_ls_hydrogen_treatment   mixed
_refine_ls_extinction_method     SHELXL
_refine_ls_extinction_coef       0.071(10)
_refine_ls_extinction_expression
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'Flack H D (1983), Acta Cryst. A39, 876-881'
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_refine_ls_restrained_S_all      1.043
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_refine_ls_shift/su_mean         0.000

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  _atom_site_fract_z
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  _atom_site_adp_type
  _atom_site_occupancy
  _atom_site_symmetry_multiplicity

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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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