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_audit_creation_method SHELXL-97

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'O8 Pb2 Te1.25 U0.75'

_chemical_formula_weight 880.40

loop_

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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'U' 'U' -9.6767 9.6646

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Pb' 'Pb' -3.3944 10.1111

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Te' 'Te' -0.5308 1.6751

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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'-x, -y, -z'

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

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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_scheme calc
_refine_ls_weighting_details
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_atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens geom
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_refine_ls_extinction_coef 0.0000(5)
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Te2 Te 0.0000 0.5000 0.0000 0.0340(13) Uani 1 2 d S . .

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Pb 0.0441(14) 0.0511(16) 0.0640(15) 0.0023(10) -0.0028(9) -0.0026(10)
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O2 0.058(18) 0.024(17) 0.031(15) 0.002(11) -0.022(14) 0.002(13)
O3 0.019(13) 0.05(2) 0.063(18) 0.031(16) 0.000(12) 0.004(12)
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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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 U1 O1 Pb 85.5(10) 1_655 4_565 ?
 Pb O1 Pb 136.0(10) 2_645 4_565 ?
 Pb O1 Pb 73.9(6) 1_554 4_565 ?
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