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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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Sr2 Sr 0.92811(4) 0.348527(11) 0.48201(4) 0.01199(7) Uani 0.8906(19) 1 d P . .

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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
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Sr2 O2 2.689(2) . ?
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 O11 Sr2 2.568(2) 2_756 ?
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