Chapter 9.11

R-TENSOR

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The program R-tensor calculates the anisotropic R tensor as described by Parkin (*Acta Cryst* (2000), **A56**, 157-162), an agreement index which is dependent on the reciprocal space directions.

The results are printed in CIF format (file *RT.CIF*) for each reflection, and a short summary file is printed to the TextServer. The only required input is a *name.FCF* file, which must be in the LIST 4 format output from SHELXL.

A sample output is :

```
Rcryst        =        0.0248
Average Reff =         0.0248
Highest Reff =         0.0294 for  -1   2  -1
Lowest  Reff =         0.0219 for   1   7   7
Axial R(h00) =         0.0261
Axial R(0k0) =         0.0261
Axial R(00l) =         0.0252
No. of data  =          3881

R-tensor in matrix form :      1.0510   -0.0871    0.2020
                              -0.0871    1.0524   -0.1431
                               0.2020   -0.1431    1.0144

Eigenvalues of R-tensor :      1.3301    0.9705    0.8172

Results written to file RT.CIF

 When using this program please quote : S. Parkin (2000), Acta Cryst, A56,
157-162
```