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C:\WINDOWS\system32\cmd.exe

Res. shift = 0.000 Å for R122      Res. sh = 0.000 for C11
uR2 = 0.8755 before cycle 0 for 17657 data and 8% / 8% parameters
Goof = 0 = 1.8721; Restricted Goof = 1.8721 for 8 restraints
Res. shift/end = 0.0000; Residuals = 0.000 for O0P      at 11:44:25
Res. shift = 0.000 Å for C0      Res. sh = 0.000 for C24
uR2 = 0.8755 before cycle 7 for 17657 data and 8% / 8% parameters
Goof = 0 = 1.8721; Restricted Goof = 1.8721 for 8 restraints
Res. shift/end = 0.0000; Residuals = -0.000 for a Goof      at 11:44:26
Res. shift = 0.000 Å for C0      Res. sh = 0.000 for C24
uR2 = 0.8755 before cycle 10 for 17657 data and 8% / 8% parameters
Goof = 0 = 1.8721; Restricted Goof = 1.8721 for 8 restraints
Res. shift/end = 0.0000; Residuals = -0.000 for O0P      at 11:44:27
Res. shift = 0.000 Å for R122      Res. sh = 0.000 for C24
uR2 = 0.8755 before cycle 11 for 17657 data and 8 / 8% parameters
Goof = 0 = 1.8721; Restricted Goof = 1.8721 for 8 restraints
R1 = 0.8279 for 14916 Fo 2-|calc|Fo| and 0.8240 for all 17657 data
uR2 = 0.8755; Goof = 0 = 1.8721; Restricted Goof = 1.8721 for all data
R1 = 0.8338 for 17657 unique reflections after merging for Fourier
Highest peak 2.32 at 0.8542 0.5975 0.4257 [ 0.00 Å from O0P ]
Deepest hole -0.74 at 0.8124 0.8572 0.4048 [ 0.74 Å from R1 ]

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+ rm_ded5265 Finished at 11:44:28 Total CPU time= 14.6 sec +
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