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C:\WINDOWS\system32\cmd.exe

Max. shift = 0.000 Å for H02      Max. dh = 0.000 for C08
u02 = 0.8056 before cycle 0 For 17653 data and 876 / 876 parameters
GsfP = 0 = 1.0941      Restrained GsfP = 1.094 for 8 restraints
Peak shift/resd = 0.000      Maximum = -0.000 for u Resd at 11:00:59
Max. shift = 0.000 Å for H03      Max. dh = 0.000 for C01
u03 = 0.8056 before cycle 7 For 17653 data and 876 / 876 parameters
GsfP = 0 = 1.0941      Restrained GsfP = 1.094 for 8 restraints
Peak shift/resd = 0.000      Maximum = -0.000 for u Resd at 11:01:01
Max. shift = 0.000 Å for H4      Max. dh = 0.000 for C09
u04 = 0.8056 before cycle 10 For 17653 data and 876 / 876 parameters
GsfP = 0 = 1.0941      Restrained GsfP = 1.094 for 8 restraints
Peak shift/resd = 0.000      Maximum = -0.000 for u Resd at 11:01:03
Max. shift = 0.000 Å for C7      Max. dh = 0.000 for C01
u07 = 0.8056 before cycle 11 For 17653 data and 0 / 876 parameters
GsfP = 0 = 1.0941      Restrained GsfP = 1.094 for 8 restraints
R0 = 0.0079 for 14915 Fo > 4sig(Po) and 0.0041 for all 17653 data
u02 = 0.8056, GsfP = 0 = 1.094, Restrained GsfP = 1.094 for all data
R0 = 0.0030 for 17653 unique reflections after merging for Fourier
Highest peak 3.31 at 0.4643 0.3635 0.4264 | 0.56 Å from H06 |
Deepest hole -0.34 at 0.5124 0.6572 0.4646 | 0.54 Å from H02 |

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* res_dif2009 finished at 11:04:00 Total CPU time 04.6 sec *
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