checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.　　　CIF dictionary　　　Interpreting this report

Datablock: _shoji9

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Bond precision:   C-C = 0.0080 A             Wavelength=0.71075

Cell:           a=10.9564(16)    b=11.3121(13)      c=14.0228(19)
                alpha=90         beta=90.834(4)     gamma=90
Temperature:    293 K

                Calculated                 Reported
Volume          1737.8(4)                  1737.8(4)
Space group     P 21/n                     P 1 21/n 1
Hall group      -P 2yn                     -P 2yn
Moiety formula  C22 H19 N O                C22 H19 N O
Sum formula     C22 H19 N O                C22 H19 N O
Mr              313.38                     313.40
Dx,g cm-3       1.198                      1.198
Z               4                          4
Mu (mm-1)       0.073                      0.073
F000            664.0                      664.0
F000'           664.26
h,k,lmax        14,14,18                   14,14,18
Nref            3974                       3959
Tmin,Tmax       0.974,0.978
Tmin'           0.950

Correction method= Not given

Data completeness= 0.996          Theta(max)= 27.430

                                  wR2(reflections)= wR= 0.1279(
R(reflections)= 0.1016( 1809)     2227)

S = 1.494               Npar= 236
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The following ALERTS were generated. Each ALERT has the format
       test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

🟡 **Alert level C**

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DIFMX01_ALERT_2_C  The maximum difference density is > 0.1*ZMAX*0.75
           _refine_diff_density_max given =      0.740
           Test value =      0.600
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
REFNR01_ALERT_3_C  Ratio of reflections to parameters is < 10 for a
           centrosymmetric structure
               sine(theta)/lambda              0.6481
               Proportion of unique data used  0.5625
               Ratio reflections to parameters 9.4364
RFACG01_ALERT_3_C  The value of the R factor is > 0.10
               R factor given   0.102
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..       46 %
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....     2.55 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density      0.74 eA-3
PLAT193_ALERT_1_C Cell and Diffraction Temperatures Differ by ....        3 Degree
PLAT230_ALERT_2_C Hirshfeld Test Diff for     C8      -- C11      ..      5.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for     C19     -- C20      ..      6.4 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C14      -- C15      ..     0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C19 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.00796 Ang.
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(7) ...... Senseless s.u.
           C(1) -H(1)        1.555   1.555 ............     #  28 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(7) ...... Senseless s.u.
           C(2) -H(2)        1.555   1.555 ............     #  29 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(7) ...... Senseless s.u.
           C(2) -H(3)        1.555   1.555 ............     #  30 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(6) ...... Senseless s.u.
           C(3) -H(4)        1.555   1.555 ............     #  31 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(6) ...... Senseless s.u.
           C(4) -H(5)        1.555   1.555 ............     #  32 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(8) ...... Senseless s.u.
           C(9) -H(6)        1.555   1.555 ............     #  33 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(8) ...... Senseless s.u.
           C(9) -H(7)        1.555   1.555 ............     #  34 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(8) ...... Senseless s.u.
           C(10)-H(8)        1.555   1.555 ............     #  35 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(8) ...... Senseless s.u.
           C(10)-H(9)        1.555   1.555 ............     #  36 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(7) ...... Senseless s.u.
           C(11)-H(10)       1.555   1.555 ............     #  37 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(7) ...... Senseless s.u.
           C(13)-H(11)       1.555   1.555 ............     #  38 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(8) ...... Senseless s.u.
           C(14)-H(12)       1.555   1.555 ............     #  39 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(9) ...... Senseless s.u.
           C(15)-H(13)       1.555   1.555 ............     #  40 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(10) ...... Senseless s.u.
           C(16)-H(14)       1.555   1.555 ............     #  41 Check
PLAT751_ALERT_4_C Bond    Calc    0.95000, Rep    0.950(8) ...... Senseless s.u.
           C(17)-H(15)       1.555   1.555 ............     #  42 Check
PLAT752_ALERT_4_C Angle   Calc     108.00, Rep    107.5(5) ...... Senseless s.u.
           C(2) -C(1) -H(1)  1.555   1.555   1.555 ....     #   38 Check
PLAT752_ALERT_4_C Angle   Calc     109.00, Rep    109.2(6) ...... Senseless s.u.
           C(9) -C(1) -H(1)  1.555   1.555   1.555 ....     #   39 Check
PLAT752_ALERT_4_C Angle   Calc     108.00, Rep    108.4(5) ...... Senseless s.u.
           C(11)-C(1) -H(1)  1.555   1.555   1.555 ....     #   40 Check
PLAT752_ALERT_4_C Angle   Calc     107.00, Rep    106.8(5) ...... Senseless s.u.
           C(1) -C(2) -H(2)  1.555   1.555   1.555 ....     #   41 Check
PLAT752_ALERT_4_C Angle   Calc     109.00, Rep    108.6(5) ...... Senseless s.u.
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                      C(1) -C(2) -H(3)       1.555   1.555   1.555 ....      #   42 Check
PLAT752_ALERT_4_C Angle   Calc      106.00, Rep    106.3(5) ......  Senseless s.u.
                      C(3) -C(2) -H(2)       1.555   1.555   1.555 ....      #   43 Check
PLAT752_ALERT_4_C Angle   Calc      108.00, Rep    108.4(5) ......  Senseless s.u.
                      C(3) -C(2) -H(3)       1.555   1.555   1.555 ....      #   44 Check
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep    109.5(6) ......  Senseless s.u.
                      H(2) -C(2) -H(3)       1.555   1.555   1.555 ....      #   45 Check
PLAT752_ALERT_4_C Angle   Calc      108.00, Rep    107.9(5) ......  Senseless s.u.
                      C(2) -C(3) -H(4)       1.555   1.555   1.555 ....      #   46 Check
PLAT752_ALERT_4_C Angle   Calc      107.00, Rep    107.4(5) ......  Senseless s.u.
                      C(4) -C(3) -H(4)       1.555   1.555   1.555 ....      #   47 Check
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep    108.6(5) ......  Senseless s.u.
                      C(12)-C(3) -H(4)       1.555   1.555   1.555 ....      #   48 Check
PLAT752_ALERT_4_C Angle   Calc      115.00, Rep    114.8(5) ......  Senseless s.u.
                      C(3) -C(4) -H(5)       1.555   1.555   1.555 ....      #   49 Check
PLAT752_ALERT_4_C Angle   Calc      116.00, Rep    116.2(5) ......  Senseless s.u.
                      C(5) -C(4) -H(5)       1.555   1.555   1.555 ....      #   50 Check
PLAT752_ALERT_4_C Angle   Calc      108.00, Rep    108.1(6) ......  Senseless s.u.
                      O(1) -C(9) -H(6)       1.555   1.555   1.555 ....      #   51 Check
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep    109.4(6) ......  Senseless s.u.
                      O(1) -C(9) -H(7)       1.555   1.555   1.555 ....      #   52 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep    109.7(6) ......  Senseless s.u.
                      C(1) -C(9) -H(6)       1.555   1.555   1.555 ....      #   53 Check
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep    108.6(5) ......  Senseless s.u.
                      C(1) -C(9) -H(7)       1.555   1.555   1.555 ....      #   54 Check
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep    109.5(7) ......  Senseless s.u.
                      H(6) -C(9) -H(7)       1.555   1.555   1.555 ....      #   55 Check
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep    109.5(6) ......  Senseless s.u.
                      O(1) -C(10)-H(8)       1.555   1.555   1.555 ....      #   56 Check
PLAT752_ALERT_4_C Angle   Calc      108.00, Rep    107.8(6) ......  Senseless s.u.
                      O(1) -C(10)-H(9)       1.555   1.555   1.555 ....      #   57 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep    109.7(5) ......  Senseless s.u.
                      C(8) -C(10)-H(8)       1.555   1.555   1.555 ....      #   58 Check
PLAT752_ALERT_4_C Angle   Calc      108.00, Rep    108.0(6) ......  Senseless s.u.
                      C(8) -C(10)-H(9)       1.555   1.555   1.555 ....      #   59 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep    109.5(7) ......  Senseless s.u.
                      H(8) -C(10)-H(9)       1.555   1.555   1.555 ....      #   60 Check
PLAT752_ALERT_4_C Angle   Calc      121.00, Rep    120.9(6) ......  Senseless s.u.
                      C(1) -C(11)-H(10)      1.555   1.555   1.555 ....      #   61 Check
PLAT752_ALERT_4_C Angle   Calc      121.00, Rep    120.6(6) ......  Senseless s.u.
                      C(8) -C(11)-H(10)      1.555   1.555   1.555 ....      #   62 Check
PLAT752_ALERT_4_C Angle   Calc      119.00, Rep    119.5(6) ......  Senseless s.u.
                      C(12)-C(13)-H(11)      1.555   1.555   1.555 ....      #   63 Check
PLAT752_ALERT_4_C Angle   Calc      120.00, Rep    120.1(6) ......  Senseless s.u.
                      C(14)-C(13)-H(11)      1.555   1.555   1.555 ....      #   64 Check
PLAT752_ALERT_4_C Angle   Calc      120.00, Rep    119.8(7) ......  Senseless s.u.
                      C(13)-C(14)-H(12)      1.555   1.555   1.555 ....      #   65 Check
PLAT752_ALERT_4_C Angle   Calc      120.00, Rep    119.6(7) ......  Senseless s.u.
                      C(15)-C(14)-H(12)      1.555   1.555   1.555 ....      #   66 Check
PLAT752_ALERT_4_C Angle   Calc      120.00, Rep    120.4(8) ......  Senseless s.u.
                      C(14)-C(15)-H(13)      1.555   1.555   1.555 ....      #   67 Check
PLAT752_ALERT_4_C Angle   Calc      119.00, Rep    119.3(8) ......  Senseless s.u.
                      C(16)-C(15)-H(13)      1.555   1.555   1.555 ....      #   68 Check
PLAT752_ALERT_4_C Angle   Calc      120.00, Rep    120.1(8) ......  Senseless s.u.
                      C(15)-C(16)-H(14)      1.555   1.555   1.555 ....      #   69 Check
PLAT752_ALERT_4_C Angle   Calc      120.00, Rep    119.5(8) ......  Senseless s.u.
                      C(17)-C(16)-H(14)      1.555   1.555   1.555 ....      #   70 Check
PLAT752_ALERT_4_C Angle   Calc      119.00, Rep    118.8(8) ......  Senseless s.u.
                      C(12)-C(17)-H(15)      1.555   1.555   1.555 ....      #   71 Check
PLAT752_ALERT_4_C Angle   Calc      120.00, Rep    120.2(7) ......  Senseless s.u.
                      C(16)-C(17)-H(15)      1.555   1.555   1.555 ....      #   72 Check
PLAT754_ALERT_4_C Contact Calc      3.23000, Rep    3.230(6) ......  Senseless s.u.
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                    O(1) -H(1)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.93000, Rep   2.928(6) ......  Senseless s.u.
                    O(1) -H(2)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.63000, Rep   2.630(5) ......  Senseless s.u.
                    O(1) -H(4)       1.555   2.545 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.08000, Rep   3.085(6) ......  Senseless s.u.
                    O(1) -H(5)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      1.95000, Rep   1.949(7) ......  Senseless s.u.
                    O(1) -H(6)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      1.96000, Rep   1.964(7) ......  Senseless s.u.
                    O(1) -H(7)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      1.95000, Rep   1.950(7) ......  Senseless s.u.
                    O(1) -H(8)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      1.93000, Rep   1.931(7) ......  Senseless s.u.
                    O(1) -H(9)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.97000, Rep   2.969(6) ......  Senseless s.u.
                    O(1) -H(10)      1.555   2.545 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.86000, Rep   2.861(6) ......  Senseless s.u.
                    O(1) -H(11)      1.555   2.545 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.61000, Rep   2.613(7) ......  Senseless s.u.
                    N(1) -H(1)       1.555   2.545 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.29000, Rep   3.285(7) ......  Senseless s.u.
                    N(1) -H(5)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.99000, Rep   2.990(8) ......  Senseless s.u.
                    N(1) -H(7)       1.555   4.444 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.55000, Rep   3.552(8) ......  Senseless s.u.
                    N(1) -H(9)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.24000, Rep   3.245(7) ......  Senseless s.u.
                    N(1) -H(10)      1.555   2.545 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.89000, Rep   2.886(7) ......  Senseless s.u.
                    N(1) -H(11)      1.555   3.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.15000, Rep   3.155(8) ......  Senseless s.u.
                    N(1) -H(12)      1.555   3.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.69000, Rep   2.685(8) ......  Senseless s.u.
                    N(1) -H(14)      1.555   4.544 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.06000, Rep   2.058(7) ......  Senseless s.u.
                    C(1) -H(2)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.08000, Rep   2.080(7) ......  Senseless s.u.
                    C(1) -H(3)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.77000, Rep   2.773(7) ......  Senseless s.u.
                    C(1) -H(4)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.03000, Rep   2.034(7) ......  Senseless s.u.
                    C(1) -H(6)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.02000, Rep   2.021(8) ......  Senseless s.u.
                    C(1) -H(7)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.34000, Rep   3.337(8) ......  Senseless s.u.
                    C(1) -H(8)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.16000, Rep   2.156(7) ......  Senseless s.u.
                    C(1) -H(10)      1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.51000, Rep   3.511(8) ......  Senseless s.u.
                    C(1) -H(14)      1.555   3.556 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.07000, Rep   2.067(7) ......  Senseless s.u.
                    C(2) -H(1)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.06000, Rep   2.056(6) ......  Senseless s.u.
                    C(2) -H(4)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.85000, Rep   2.847(6) ......  Senseless s.u.
                    C(2) -H(5)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.70000, Rep   2.704(7) ......  Senseless s.u.
                    C(2) -H(6)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.38000, Rep   3.379(8) ......  Senseless s.u.
                    C(2) -H(7)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.95000, Rep   2.946(7) ......  Senseless s.u.
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                    C(2) -H(10)      1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.76000, Rep   2.758(9) ......  Senseless s.u.
                    C(2) -H(15)      1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.33000, Rep   3.333(7) ......  Senseless s.u.
                    C(3) -H(1)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.04000, Rep   2.038(6) ......  Senseless s.u.
                    C(3) -H(2)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.06000, Rep   2.063(6) ......  Senseless s.u.
                    C(3) -H(3)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.10000, Rep   2.099(6) ......  Senseless s.u.
                    C(3) -H(5)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.12000, Rep   3.117(7) ......  Senseless s.u.
                    C(3) -H(10)      1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.64000, Rep   2.637(7) ......  Senseless s.u.
                    C(3) -H(11)      1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.74000, Rep   2.739(8) ......  Senseless s.u.
                    C(3) -H(15)      1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.66000, Rep   2.664(7) ......  Senseless s.u.
                    C(4) -H(2)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.36000, Rep   3.363(6) ......  Senseless s.u.
                    C(4) -H(3)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.01000, Rep   2.014(6) ......  Senseless s.u.
                    C(4) -H(4)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.15000, Rep   3.153(7) ......  Senseless s.u.
                    C(4) -H(9)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.10000, Rep   3.102(6) ......  Senseless s.u.
                    C(4) -H(10)      1.555  2.545 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.32000, Rep   3.318(7) ......  Senseless s.u.
                    C(4) -H(11)      1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.32000, Rep   3.320(8) ......  Senseless s.u.
                    C(4) -H(15)      1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.64000, Rep   2.638(6) ......  Senseless s.u.
                    C(5) -H(4)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    1.95000, Rep   1.946(7) ......  Senseless s.u.
                    C(5) -H(5)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.66000, Rep   2.664(7) ......  Senseless s.u.
                    C(5) -H(9)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.48000, Rep   3.478(7) ......  Senseless s.u.
                    C(5) -H(10)      1.555  2.545 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.85000, Rep   2.850(7) ......  Senseless s.u.
                    C(6) -H(4)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.35000, Rep   3.350(7) ......  Senseless s.u.
                    C(6) -H(5)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.53000, Rep   3.533(7) ......  Senseless s.u.
                    C(6) -H(6)       1.555  2.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.86000, Rep   2.859(7) ......  Senseless s.u.
                    C(6) -H(9)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.57000, Rep   3.569(7) ......  Senseless s.u.
                    C(6) -H(10)      1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.08000, Rep   3.075(8) ......  Senseless s.u.
                    C(7) -H(4)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.07000, Rep   3.073(8) ......  Senseless s.u.
                    C(7) -H(8)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.56000, Rep   2.560(7) ......  Senseless s.u.
                    C(7) -H(9)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.68000, Rep   2.684(7) ......  Senseless s.u.
                    C(7) -H(10)      1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    3.16000, Rep   3.157(8) ......  Senseless s.u.
                    C(8) -H(1)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.87000, Rep   2.867(7) ......  Senseless s.u.
                    C(8) -H(4)       1.555  1.555 .............    #   46 Check
PLAT754_ALERT_4_C Contact Calc    2.97000, Rep   2.968(8) ......  Senseless s.u.
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                      C(8) -H(7)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.05000, Rep    2.055(7) ......   Senseless s.u.
                      C(8) -H(8)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.03000, Rep    2.035(7) ......   Senseless s.u.
                      C(8) -H(9)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     1.99000, Rep    1.993(7) ......   Senseless s.u.
                      C(8) -H(10)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.12000, Rep    3.118(8) ......   Senseless s.u.
                      C(8) -H(13)        1.555   1.655 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.03000, Rep    2.028(7) ......   Senseless s.u.
                      C(9) -H(1)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.52000, Rep    2.519(8) ......   Senseless s.u.
                      C(9) -H(2)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.25000, Rep    3.254(7) ......   Senseless s.u.
                      C(9) -H(3)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.61000, Rep    2.614(8) ......   Senseless s.u.
                      C(9) -H(8)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.14000, Rep    3.144(8) ......   Senseless s.u.
                      C(9) -H(9)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.33000, Rep    3.328(7) ......   Senseless s.u.
                      C(9) -H(10)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.27000, Rep    3.271(7) ......   Senseless s.u.
                      C(9) -H(11)        1.555   2.545 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.37000, Rep    3.372(7) ......   Senseless s.u.
                      C(10)-H(4)         1.555   2.545 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.58000, Rep    3.580(7) ......   Senseless s.u.
                      C(10)-H(5)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.15000, Rep    3.148(8) ......   Senseless s.u.
                      C(10)-H(6)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.50000, Rep    2.504(8) ......   Senseless s.u.
                      C(10)-H(7)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.35000, Rep    3.350(7) ......   Senseless s.u.
                      C(10)-H(10)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.25000, Rep    3.251(7) ......   Senseless s.u.
                      C(10)-H(11)        1.555   2.545 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.49000, Rep    3.488(9) ......   Senseless s.u.
                      C(10)-H(13)        1.555   1.655 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.02000, Rep    2.020(7) ......   Senseless s.u.
                      C(11)-H(1)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.17000, Rep    3.174(7) ......   Senseless s.u.
                      C(11)-H(2)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.97000, Rep    2.974(7) ......   Senseless s.u.
                      C(11)-H(3)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.39000, Rep    2.393(7) ......   Senseless s.u.
                      C(11)-H(4)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.26000, Rep    3.258(6) ......   Senseless s.u.
                      C(11)-H(5)         1.555   2.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.30000, Rep    3.297(7) ......   Senseless s.u.
                      C(11)-H(6)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.72000, Rep    2.722(7) ......   Senseless s.u.
                      C(11)-H(7)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.94000, Rep    2.943(7) ......   Senseless s.u.
                      C(11)-H(8)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.19000, Rep    3.193(7) ......   Senseless s.u.
                      C(11)-H(9)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.08000, Rep    3.080(8) ......   Senseless s.u.
                      C(11)-H(13)        1.555   1.655 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.78000, Rep    2.783(7) ......   Senseless s.u.
                      C(12)-H(2)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.62000, Rep    2.617(7) ......   Senseless s.u.
                      C(12)-H(3)         1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.04000, Rep    2.042(7) ......   Senseless s.u.
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                    C(12)-H(4)         1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.70000, Rep    2.702(6) ......    Senseless s.u.
                    C(12)-H(5)         1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.03000, Rep    2.028(7) ......    Senseless s.u.
                    C(12)-H(11)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.26000, Rep    3.261(8) ......    Senseless s.u.
                    C(12)-H(12)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.26000, Rep    3.261(9) ......    Senseless s.u.
                    C(12)-H(14)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.03000, Rep    2.028(7) ......    Senseless s.u.
                    C(12)-H(15)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.55000, Rep    2.552(7) ......    Senseless s.u.
                    C(13)-H(4)         1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.18000, Rep    3.179(7) ......    Senseless s.u.
                    C(13)-H(8)         1.555   2.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.03000, Rep    2.034(8) ......    Senseless s.u.
                    C(13)-H(12)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.24000, Rep    3.237(9) ......    Senseless s.u.
                    C(13)-H(13)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.23000, Rep    3.229(7) ......    Senseless s.u.
                    C(13)-H(15)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.04000, Rep    2.037(9) ......    Senseless s.u.
                    C(14)-H(11)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.00000, Rep    2.004(9) ......    Senseless s.u.
                    C(14)-H(13)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.20000, Rep    3.198(9) ......    Senseless s.u.
                    C(14)-H(14)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.42000, Rep    3.416(9) ......    Senseless s.u.
                    C(15)-H(8)         1.555   1.455 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.23000, Rep    3.230(9) ......    Senseless s.u.
                    C(15)-H(11)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.00000, Rep    1.997(9) ......    Senseless s.u.
                    C(15)-H(12)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.00000, Rep    2.003(10) ......   Senseless s.u.
                    C(15)-H(14)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.22000, Rep    3.221(9) ......    Senseless s.u.
                    C(15)-H(15)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.38000, Rep    3.377(9) ......    Senseless s.u.
                    C(16)-H(1)         1.555   3.556 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.55000, Rep    3.552(8) ......    Senseless s.u.
                    C(16)-H(3)         1.555   3.556 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.20000, Rep    3.196(9) ......    Senseless s.u.
                    C(16)-H(12)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.33000, Rep    3.326(9) ......    Senseless s.u.
                    C(16)-H(12)        1.555   2.445 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.00000, Rep    1.996(10) ......   Senseless s.u.
                    C(16)-H(13)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.03000, Rep    2.027(10) ......   Senseless s.u.
                    C(16)-H(15)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.87000, Rep    2.873(9) ......    Senseless s.u.
                    C(17)-H(2)         1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     2.97000, Rep    2.975(9) ......    Senseless s.u.
                    C(17)-H(3)         1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.44000, Rep    3.441(8) ......    Senseless s.u.
                    C(17)-H(3)         1.555   3.556 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.30000, Rep    3.303(8) ......    Senseless s.u.
                    C(17)-H(4)         1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.12000, Rep    3.118(8) ......    Senseless s.u.
                    C(17)-H(5)         1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.24000, Rep    3.235(7) ......    Senseless s.u.
                    C(17)-H(11)        1.555   1.555 ............      #    46 Check
PLAT754_ALERT_4_C Contact Calc     3.40000, Rep    3.403(8) ......    Senseless s.u.
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                     C(17)-H(12)         1.555   2.445 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.22000, Rep    3.219(9) ......  Senseless s.u.
                     C(17)-H(13)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.02000, Rep    2.020(10) ......  Senseless s.u.
                     C(17)-H(14)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.26000, Rep    3.257(8) ......  Senseless s.u.
                     C(18)-H(6)          1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.02000, Rep    3.024(10) ......  Senseless s.u.
                     C(19)-H(6)          1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.37000, Rep    3.371(12) ......  Senseless s.u.
                     C(19)-H(8)          1.555   3.655 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.12000, Rep    3.119(9) ......  Senseless s.u.
                     C(20)-H(2)          1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.14000, Rep    3.141(11) ......  Senseless s.u.
                     C(20)-H(6)          1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.16000, Rep    3.163(11) ......  Senseless s.u.
                     C(20)-H(8)          1.555   3.655 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.22000, Rep    3.217(12) ......  Senseless s.u.
                     C(20)-H(9)          1.555   3.655 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.19000, Rep    3.189(8) ......  Senseless s.u.
                     C(21)-H(2)          1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.45000, Rep    3.446(9) ......  Senseless s.u.
                     C(21)-H(6)          1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.19000, Rep    3.185(9) ......  Senseless s.u.
                     C(21)-H(10)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.51000, Rep    3.515(8) ......  Senseless s.u.
                     C(21)-H(15)         1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.28000, Rep    3.283(7) ......  Senseless s.u.
                     C(22)-H(1)          1.555   2.545 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.44000, Rep    2.443(7) ......  Senseless s.u.
                     C(22)-H(5)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.94000, Rep    2.940(8) ......  Senseless s.u.
                     C(22)-H(9)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.08000, Rep    3.082(7) ......  Senseless s.u.
                     C(22)-H(10)         1.555   2.545 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.39000, Rep    3.393(7) ......  Senseless s.u.
                     C(22)-H(11)         1.555   3.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.23000, Rep    3.230(6) ......  Senseless s.u.
                     H(1) -O(1)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.61000, Rep    2.613(7) ......  Senseless s.u.
                     H(1) -N(1)          1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.07000, Rep    2.067(7) ......  Senseless s.u.
                     H(1) -C(2)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.33000, Rep    3.333(7) ......  Senseless s.u.
                     H(1) -C(3)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.16000, Rep    3.157(8) ......  Senseless s.u.
                     H(1) -C(8)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.03000, Rep    2.028(7) ......  Senseless s.u.
                     H(1) -C(9)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.02000, Rep    2.020(7) ......  Senseless s.u.
                     H(1) -C(11)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.38000, Rep    3.377(9) ......  Senseless s.u.
                     H(1) -C(16)         1.555   3.556 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.28000, Rep    3.283(7) ......  Senseless s.u.
                     H(1) -C(22)         1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.58000, Rep    2.577(7) ......  Senseless s.u.
                     H(1) -H(2)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.17000, Rep    2.169(7) ......  Senseless s.u.
                     H(1) -H(3)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.36000, Rep    3.357(7) ......  Senseless s.u.
                     H(1) -H(4)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.37000, Rep    2.369(7) ......  Senseless s.u.
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                          H(1) -H(6)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.25000, Rep    2.255(7) ......   Senseless s.u.
                          H(1) -H(7)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.34000, Rep    2.342(7) ......   Senseless s.u.
                          H(1) -H(10)       1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.70000, Rep    2.699(9) ......   Senseless s.u.
                          H(1) -H(14)       1.555   3.556 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.93000, Rep    2.928(6) ......   Senseless s.u.
                          H(2) -O(1)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.06000, Rep    2.058(7) ......   Senseless s.u.
                          H(2) -C(1)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.04000, Rep    2.038(6) ......   Senseless s.u.
                          H(2) -C(3)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.66000, Rep    2.664(7) ......   Senseless s.u.
                          H(2) -C(4)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.52000, Rep    2.519(8) ......   Senseless s.u.
                          H(2) -C(9)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.17000, Rep    3.174(7) ......   Senseless s.u.
                          H(2) -C(11)       1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.78000, Rep    2.783(7) ......   Senseless s.u.
                          H(2) -C(12)       1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.87000, Rep    2.873(9) ......   Senseless s.u.
                          H(2) -C(17)       1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.12000, Rep    3.119(9) ......   Senseless s.u.
                          H(2) -C(20)       1.555   2.545 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.19000, Rep    3.189(8) ......   Senseless s.u.
                          H(2) -C(21)       1.555   2.545 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.58000, Rep    2.577(7) ......   Senseless s.u.
                          H(2) -H(1)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      1.55000, Rep    1.551(7) ......   Senseless s.u.
                          H(2) -H(3)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.78000, Rep    2.781(6) ......   Senseless s.u.
                          H(2) -H(4)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.59000, Rep    2.593(7) ......   Senseless s.u.
                          H(2) -H(5)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.35000, Rep    2.352(8) ......   Senseless s.u.
                          H(2) -H(6)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.42000, Rep    3.419(8) ......   Senseless s.u.
                          H(2) -H(7)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.34000, Rep    2.335(9) ......   Senseless s.u.
                          H(2) -H(15)       1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.08000, Rep    2.080(7) ......   Senseless s.u.
                          H(3) -C(1)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.06000, Rep    2.063(6) ......   Senseless s.u.
                          H(3) -C(3)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.36000, Rep    3.363(6) ......   Senseless s.u.
                          H(3) -C(4)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.25000, Rep    3.254(7) ......   Senseless s.u.
                          H(3) -C(9)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.97000, Rep    2.974(7) ......   Senseless s.u.
                          H(3) -C(11)       1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.62000, Rep    2.617(7) ......   Senseless s.u.
                          H(3) -C(12)       1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.55000, Rep    3.552(8) ......   Senseless s.u.
                          H(3) -C(16)       1.555   3.556 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.97000, Rep    2.975(9) ......   Senseless s.u.
                          H(3) -C(17)       1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.44000, Rep    3.441(8) ......   Senseless s.u.
                          H(3) -C(17)       1.555   3.556 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.17000, Rep    2.169(7) ......   Senseless s.u.
                          H(3) -H(1)        1.555   1.555 ............     #   46 Check
PLAT754_ALERT_4_C Contact Calc      1.55000, Rep    1.551(7) ......   Senseless s.u.
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              H(3)  -H(2)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.41000, Rep    2.407(6) ......  Senseless s.u.
              H(3)  -H(4)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.28000, Rep    3.277(7) ......  Senseless s.u.
              H(3)  -H(6)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.47000, Rep    3.474(7) ......  Senseless s.u.
              H(3)  -H(9)          1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.20000, Rep    3.201(7) ......  Senseless s.u.
              H(3)  -H(10)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.24000, Rep    3.239(8) ......  Senseless s.u.
              H(3)  -H(14)         1.555   3.556 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.77000, Rep    2.774(8) ......  Senseless s.u.
              H(3)  -H(15)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.03000, Rep    3.032(8) ......  Senseless s.u.
              H(3)  -H(15)         1.555   3.556 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.63000, Rep    2.630(5) ......  Senseless s.u.
              H(4)  -O(1)          1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.77000, Rep    2.773(7) ......  Senseless s.u.
              H(4)  -C(1)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.06000, Rep    2.056(6) ......  Senseless s.u.
              H(4)  -C(2)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.01000, Rep    2.014(6) ......  Senseless s.u.
              H(4)  -C(4)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.64000, Rep    2.638(6) ......  Senseless s.u.
              H(4)  -C(5)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.85000, Rep    2.850(7) ......  Senseless s.u.
              H(4)  -C(6)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.08000, Rep    3.075(8) ......  Senseless s.u.
              H(4)  -C(7)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.87000, Rep    2.867(7) ......  Senseless s.u.
              H(4)  -C(8)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.37000, Rep    3.372(7) ......  Senseless s.u.
              H(4)  -C(10)         1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.39000, Rep    2.393(7) ......  Senseless s.u.
              H(4)  -C(11)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.04000, Rep    2.042(7) ......  Senseless s.u.
              H(4)  -C(12)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.55000, Rep    2.552(7) ......  Senseless s.u.
              H(4)  -C(13)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.30000, Rep    3.303(8) ......  Senseless s.u.
              H(4)  -C(17)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.36000, Rep    3.357(7) ......  Senseless s.u.
              H(4)  -H(1)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.78000, Rep    2.781(6) ......  Senseless s.u.
              H(4)  -H(2)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.41000, Rep    2.407(6) ......  Senseless s.u.
              H(4)  -H(3)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.82000, Rep    2.821(6) ......  Senseless s.u.
              H(4)  -H(5)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.51000, Rep    3.512(7) ......  Senseless s.u.
              H(4)  -H(8)          1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.25000, Rep    3.244(7) ......  Senseless s.u.
              H(4)  -H(9)          1.555   2.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.52000, Rep    2.515(7) ......  Senseless s.u.
              H(4)  -H(10)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.35000, Rep    2.350(7) ......  Senseless s.u.
              H(4)  -H(11)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.59000, Rep    3.591(8) ......  Senseless s.u.
              H(4)  -H(15)         1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.08000, Rep    3.085(6) ......  Senseless s.u.
              H(5)  -O(1)          1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.29000, Rep    3.285(7) ......  Senseless s.u.
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                    H(5)  -N(1)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      2.85000, Rep    2.847(6) ......  Senseless s.u.
                    H(5)  -C(2)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      2.10000, Rep    2.099(6) ......  Senseless s.u.
                    H(5)  -C(3)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      1.95000, Rep    1.946(7) ......  Senseless s.u.
                    H(5)  -C(5)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.35000, Rep    3.350(7) ......  Senseless s.u.
                    H(5)  -C(6)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.58000, Rep    3.580(7) ......  Senseless s.u.
                    H(5)  -C(10)        1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.26000, Rep    3.258(6) ......  Senseless s.u.
                    H(5)  -C(11)        1.555   2.545 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      2.70000, Rep    2.702(6) ......  Senseless s.u.
                    H(5)  -C(12)        1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.12000, Rep    3.118(8) ......  Senseless s.u.
                    H(5)  -C(17)        1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      2.44000, Rep    2.443(7) ......  Senseless s.u.
                    H(5)  -C(22)        1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      2.59000, Rep    2.593(7) ......  Senseless s.u.
                    H(5)  -H(2)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      2.82000, Rep    2.821(6) ......  Senseless s.u.
                    H(5)  -H(4)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.41000, Rep    3.412(7) ......  Senseless s.u.
                    H(5)  -H(9)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      2.34000, Rep    2.344(6) ......  Senseless s.u.
                    H(5)  -H(10)        1.555   2.545 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      2.99000, Rep    2.994(8) ......  Senseless s.u.
                    H(5)  -H(15)        1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      1.95000, Rep    1.949(7) ......  Senseless s.u.
                    H(6)  -O(1)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      2.03000, Rep    2.034(7) ......  Senseless s.u.
                    H(6)  -C(1)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      2.70000, Rep    2.704(7) ......  Senseless s.u.
                    H(6)  -C(2)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.53000, Rep    3.533(7) ......  Senseless s.u.
                    H(6)  -C(6)         1.555   2.545 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.15000, Rep    3.148(8) ......  Senseless s.u.
                    H(6)  -C(10)        1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.30000, Rep    3.297(7) ......  Senseless s.u.
                    H(6)  -C(11)        1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.26000, Rep    3.257(8) ......  Senseless s.u.
                    H(6)  -C(18)        1.555   2.545 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.02000, Rep    3.024(10) ......  Senseless s.u.
                    H(6)  -C(19)        1.555   2.545 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.14000, Rep    3.141(11) ......  Senseless s.u.
                    H(6)  -C(20)        1.555   2.545 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.45000, Rep    3.446(9) ......  Senseless s.u.
                    H(6)  -C(21)        1.555   2.545 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      2.37000, Rep    2.369(7) ......  Senseless s.u.
                    H(6)  -H(1)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      2.35000, Rep    2.352(8) ......  Senseless s.u.
                    H(6)  -H(2)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.28000, Rep    3.277(7) ......  Senseless s.u.
                    H(6)  -H(3)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      1.55000, Rep    1.551(8) ......  Senseless s.u.
                    H(6)  -H(7)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.43000, Rep    3.427(8) ......  Senseless s.u.
                    H(6)  -H(8)         1.555   1.555 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      3.42000, Rep    3.423(8) ......  Senseless s.u.
                    H(6)  -H(11)        1.555   2.545 ............        #    46 Check
      PLAT754_ALERT_4_C Contact Calc      1.96000, Rep    1.964(7) ......  Senseless s.u.
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                      H(7) -O(1)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.99000, Rep    2.990(8) ......  Senseless s.u.
                      H(7) -N(1)        1.555   4.545 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.02000, Rep    2.021(8) ......  Senseless s.u.
                      H(7) -C(1)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.38000, Rep    3.379(8) ......  Senseless s.u.
                      H(7) -C(2)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.97000, Rep    2.968(8) ......  Senseless s.u.
                      H(7) -C(8)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.50000, Rep    2.504(8) ......  Senseless s.u.
                      H(7) -C(10)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.72000, Rep    2.722(7) ......  Senseless s.u.
                      H(7) -C(11)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.25000, Rep    2.255(7) ......  Senseless s.u.
                      H(7) -H(1)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.42000, Rep    3.419(8) ......  Senseless s.u.
                      H(7) -H(2)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     1.55000, Rep    1.551(8) ......  Senseless s.u.
                      H(7) -H(6)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.42000, Rep    2.421(8) ......  Senseless s.u.
                      H(7) -H(8)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.40000, Rep    3.397(8) ......  Senseless s.u.
                      H(7) -H(9)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.47000, Rep    3.469(7) ......  Senseless s.u.
                      H(7) -H(10)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.93000, Rep    2.932(7) ......  Senseless s.u.
                      H(7) -H(11)       1.555   2.545 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.10000, Rep    3.101(9) ......  Senseless s.u.
                      H(7) -H(13)       1.555   1.655 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.96000, Rep    2.963(9) ......  Senseless s.u.
                      H(7) -H(14)       1.555   1.655 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     1.95000, Rep    1.950(7) ......  Senseless s.u.
                      H(8) -O(1)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.34000, Rep    3.337(8) ......  Senseless s.u.
                      H(8) -C(1)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.07000, Rep    3.073(8) ......  Senseless s.u.
                      H(8) -C(7)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.05000, Rep    2.055(7) ......  Senseless s.u.
                      H(8) -C(8)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.61000, Rep    2.614(8) ......  Senseless s.u.
                      H(8) -C(9)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.94000, Rep    2.943(7) ......  Senseless s.u.
                      H(8) -C(11)       1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.18000, Rep    3.179(7) ......  Senseless s.u.
                      H(8) -C(13)       1.555   2.545 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.42000, Rep    3.416(9) ......  Senseless s.u.
                      H(8) -C(15)       1.555   1.655 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.37000, Rep    3.371(12) ......  Senseless s.u.
                      H(8) -C(19)       1.555   3.655 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.16000, Rep    3.163(11) ......  Senseless s.u.
                      H(8) -C(20)       1.555   3.655 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.51000, Rep    3.512(7) ......  Senseless s.u.
                      H(8) -H(4)        1.555   2.545 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.43000, Rep    3.427(8) ......  Senseless s.u.
                      H(8) -H(6)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.42000, Rep    2.421(8) ......  Senseless s.u.
                      H(8) -H(7)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     1.55000, Rep    1.551(8) ......  Senseless s.u.
                      H(8) -H(9)        1.555   1.555 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.78000, Rep    2.783(7) ......  Senseless s.u.
                      H(8) -H(11)       1.555   2.545 ............      #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.96000, Rep    2.964(9) ......  Senseless s.u.
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                              H(8) -H(13)        1.555   1.655 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.50000, Rep    3.500(9) ......   Senseless s.u.
                              H(8) -H(14)        1.555   1.655 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      1.93000, Rep    1.931(7) ......   Senseless s.u.
                              H(9) -O(1)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.55000, Rep    3.552(8) ......   Senseless s.u.
                              H(9) -N(1)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.15000, Rep    3.153(7) ......   Senseless s.u.
                              H(9) -C(4)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      2.66000, Rep    2.664(7) ......   Senseless s.u.
                              H(9) -C(5)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      2.86000, Rep    2.859(7) ......   Senseless s.u.
                              H(9) -C(6)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      2.56000, Rep    2.560(7) ......   Senseless s.u.
                              H(9) -C(7)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      2.03000, Rep    2.035(7) ......   Senseless s.u.
                              H(9) -C(8)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.14000, Rep    3.144(8) ......   Senseless s.u.
                              H(9) -C(9)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.19000, Rep    3.193(7) ......   Senseless s.u.
                              H(9) -C(11)        1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.22000, Rep    3.217(12) ......  Senseless s.u.
                              H(9) -C(20)        1.555   3.655 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      2.94000, Rep    2.940(8) ......   Senseless s.u.
                              H(9) -C(22)        1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.47000, Rep    3.474(7) ......   Senseless s.u.
                              H(9) -H(3)         1.555   2.545 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.25000, Rep    3.244(7) ......   Senseless s.u.
                              H(9) -H(4)         1.555   2.545 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.41000, Rep    3.412(7) ......   Senseless s.u.
                              H(9) -H(5)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.40000, Rep    3.397(8) ......   Senseless s.u.
                              H(9) -H(7)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      1.55000, Rep    1.551(8) ......   Senseless s.u.
                              H(9) -H(8)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.42000, Rep    3.422(7) ......   Senseless s.u.
                              H(9) -H(10)        1.555   2.545 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.59000, Rep    3.591(7) ......   Senseless s.u.
                              H(9) -H(11)        1.555   2.545 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      2.97000, Rep    2.969(6) ......   Senseless s.u.
                              H(10)-O(1)         1.555   2.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.24000, Rep    3.245(7) ......   Senseless s.u.
                              H(10)-N(1)         1.555   2.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      2.16000, Rep    2.156(7) ......   Senseless s.u.
                              H(10)-C(1)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      2.95000, Rep    2.946(7) ......   Senseless s.u.
                              H(10)-C(2)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.12000, Rep    3.117(7) ......   Senseless s.u.
                              H(10)-C(3)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.10000, Rep    3.102(6) ......   Senseless s.u.
                              H(10)-C(4)         1.555   2.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.48000, Rep    3.478(7) ......   Senseless s.u.
                              H(10)-C(5)         1.555   2.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.57000, Rep    3.569(7) ......   Senseless s.u.
                              H(10)-C(6)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      2.68000, Rep    2.684(7) ......   Senseless s.u.
                              H(10)-C(7)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      1.99000, Rep    1.993(7) ......   Senseless s.u.
                              H(10)-C(8)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.33000, Rep    3.328(7) ......   Senseless s.u.
                              H(10)-C(9)         1.555   1.555 ............      #   46 Check
          PLAT754_ALERT_4_C Contact Calc      3.35000, Rep    3.350(7) ......   Senseless s.u.
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                        H(10)-C(10)        1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.19000, Rep    3.185(9) ......    Senseless s.u.
                        H(10)-C(21)        1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.08000, Rep    3.082(7) ......    Senseless s.u.
                        H(10)-C(22)        1.555   2.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.34000, Rep    2.342(7) ......    Senseless s.u.
                        H(10)-H(1)         1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.20000, Rep    3.201(7) ......    Senseless s.u.
                        H(10)-H(3)         1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.52000, Rep    2.515(7) ......    Senseless s.u.
                        H(10)-H(4)         1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.34000, Rep    2.344(6) ......    Senseless s.u.
                        H(10)-H(5)         1.555   2.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.47000, Rep    3.469(7) ......    Senseless s.u.
                        H(10)-H(7)         1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.42000, Rep    3.422(7) ......    Senseless s.u.
                        H(10)-H(9)         1.555   2.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.17000, Rep    3.168(8) ......    Senseless s.u.
                        H(10)-H(13)        1.555   1.655 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.86000, Rep    2.861(6) ......    Senseless s.u.
                        H(11)-O(1)         1.555   2.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.89000, Rep    2.886(7) ......    Senseless s.u.
                        H(11)-N(1)         1.555   3.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.64000, Rep    2.637(7) ......    Senseless s.u.
                        H(11)-C(3)         1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.32000, Rep    3.318(7) ......    Senseless s.u.
                        H(11)-C(4)         1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.27000, Rep    3.271(7) ......    Senseless s.u.
                        H(11)-C(9)         1.555   2.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.25000, Rep    3.251(7) ......    Senseless s.u.
                        H(11)-C(10)        1.555   2.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.03000, Rep    2.028(7) ......    Senseless s.u.
                        H(11)-C(12)        1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.04000, Rep    2.037(9) ......    Senseless s.u.
                        H(11)-C(14)        1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.23000, Rep    3.230(9) ......    Senseless s.u.
                        H(11)-C(15)        1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.24000, Rep    3.235(7) ......    Senseless s.u.
                        H(11)-C(17)        1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.39000, Rep    3.393(7) ......    Senseless s.u.
                        H(11)-C(22)        1.555   3.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.35000, Rep    2.350(7) ......    Senseless s.u.
                        H(11)-H(4)         1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.42000, Rep    3.423(8) ......    Senseless s.u.
                        H(11)-H(6)         1.555   2.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.93000, Rep    2.932(7) ......    Senseless s.u.
                        H(11)-H(7)         1.555   2.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.78000, Rep    2.783(7) ......    Senseless s.u.
                        H(11)-H(8)         1.555   2.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.59000, Rep    3.591(7) ......    Senseless s.u.
                        H(11)-H(9)         1.555   2.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.34000, Rep    2.336(9) ......    Senseless s.u.
                        H(11)-H(12)        1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.15000, Rep    3.155(8) ......    Senseless s.u.
                        H(12)-N(1)         1.555   3.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.26000, Rep    3.261(8) ......    Senseless s.u.
                        H(12)-C(12)        1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.03000, Rep    2.034(8) ......    Senseless s.u.
                        H(12)-C(13)        1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       2.00000, Rep    1.997(9) ......    Senseless s.u.
                        H(12)-C(15)        1.555   1.555 .............     #    46 Check
PLAT754_ALERT_4_C Contact Calc       3.20000, Rep    3.196(9) ......    Senseless s.u.
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                        H(12)-C(16)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.33000, Rep   3.326(9) ......   Senseless s.u.
                        H(12)-C(16)        1.555   2.455 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.40000, Rep   3.403(8) ......   Senseless s.u.
                        H(12)-C(17)        1.555   2.455 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.34000, Rep   2.336(9) ......   Senseless s.u.
                        H(12)-H(11)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.30000, Rep   2.298(9) ......   Senseless s.u.
                        H(12)-H(13)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.02000, Rep   3.020(9) ......   Senseless s.u.
                        H(12)-H(14)        1.555   2.455 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.17000, Rep   3.172(8) ......   Senseless s.u.
                        H(12)-H(15)        1.555   2.455 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.12000, Rep   3.118(8) ......   Senseless s.u.
                        H(13)-C(8)         1.555   1.455 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.49000, Rep   3.488(9) ......   Senseless s.u.
                        H(13)-C(10)        1.555   1.455 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.08000, Rep   3.080(8) ......   Senseless s.u.
                        H(13)-C(11)        1.555   1.455 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.24000, Rep   3.237(9) ......   Senseless s.u.
                        H(13)-C(13)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.00000, Rep   2.004(9) ......   Senseless s.u.
                        H(13)-C(14)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.00000, Rep   1.996(10) ......   Senseless s.u.
                        H(13)-C(16)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.22000, Rep   3.219(9) ......   Senseless s.u.
                        H(13)-C(17)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.10000, Rep   3.101(9) ......   Senseless s.u.
                        H(13)-H(7)         1.555   1.455 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.96000, Rep   2.964(9) ......   Senseless s.u.
                        H(13)-H(8)         1.555   1.455 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.17000, Rep   3.168(8) ......   Senseless s.u.
                        H(13)-H(10)        1.555   1.455 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.30000, Rep   2.298(9) ......   Senseless s.u.
                        H(13)-H(12)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.29000, Rep   2.292(10) ......   Senseless s.u.
                        H(13)-H(14)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.69000, Rep   2.685(8) ......   Senseless s.u.
                        H(14)-N(1)         1.555   4.445 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.51000, Rep   3.511(8) ......   Senseless s.u.
                        H(14)-C(1)         1.555   3.556 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.26000, Rep   3.261(9) ......   Senseless s.u.
                        H(14)-C(12)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.20000, Rep   3.198(9) ......   Senseless s.u.
                        H(14)-C(14)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.00000, Rep   2.003(10) ......   Senseless s.u.
                        H(14)-C(15)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.02000, Rep   2.020(10) ......   Senseless s.u.
                        H(14)-C(17)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.70000, Rep   2.699(9) ......   Senseless s.u.
                        H(14)-H(1)         1.555   3.556 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.24000, Rep   3.239(8) ......   Senseless s.u.
                        H(14)-H(3)         1.555   3.556 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.96000, Rep   2.963(9) ......   Senseless s.u.
                        H(14)-H(7)         1.555   1.455 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.50000, Rep   3.500(9) ......   Senseless s.u.
                        H(14)-H(8)         1.555   1.455 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      3.02000, Rep   3.020(9) ......   Senseless s.u.
                        H(14)-H(12)        1.555   2.445 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.29000, Rep   2.292(10) ......   Senseless s.u.
                        H(14)-H(13)        1.555   1.555 ............        #   46 Check
PLAT754_ALERT_4_C Contact Calc      2.32000, Rep   2.321(10) ......   Senseless s.u.
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                     H(14)-H(15)       1.555  1.555 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.76000, Rep   2.758(9) ......  Senseless s.u.
                     H(15)-C(2)        1.555  1.555 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.74000, Rep   2.739(8) ......  Senseless s.u.
                     H(15)-C(3)        1.555  1.555 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.32000, Rep   3.320(8) ......  Senseless s.u.
                     H(15)-C(4)        1.555  1.555 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.03000, Rep   2.028(7) ......  Senseless s.u.
                     H(15)-C(12)       1.555  1.555 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.23000, Rep   3.229(7) ......  Senseless s.u.
                     H(15)-C(13)       1.555  1.555 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.22000, Rep   3.221(9) ......  Senseless s.u.
                     H(15)-C(15)       1.555  1.555 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.03000, Rep   2.027(10) ......  Senseless s.u.
                     H(15)-C(16)       1.555  1.555 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.51000, Rep   3.515(8) ......  Senseless s.u.
                     H(15)-C(21)       1.555  2.545 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.34000, Rep   2.335(9) ......  Senseless s.u.
                     H(15)-H(2)        1.555  1.555 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.77000, Rep   2.774(8) ......  Senseless s.u.
                     H(15)-H(3)        1.555  1.555 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.03000, Rep   3.032(8) ......  Senseless s.u.
                     H(15)-H(3)        1.555  3.556 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.59000, Rep   3.591(8) ......  Senseless s.u.
                     H(15)-H(4)        1.555  1.555 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.99000, Rep   2.994(8) ......  Senseless s.u.
                     H(15)-H(5)        1.555  1.555 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     3.17000, Rep   3.172(8) ......  Senseless s.u.
                     H(15)-H(12)       1.555  2.445 ............    #   46 Check
PLAT754_ALERT_4_C Contact Calc     2.32000, Rep   2.321(10) ......  Senseless s.u.
                     H(15)-H(14)       1.555  1.555 ............    #   46 Check
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⬤ Alert level G

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CHEMS02_ALERT_1_G  Please check that you have entered the correct
            _publ_requested_category classification of your compound;
            FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
            FO or CO or EO for organic.
            From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or
            From the CIF: _chemical_formula_sum:C22 H19 N1 O1
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....      0.70 mm
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)      293 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       21 Do !
        C(4)-C(5)-C(22-N(1) -145.00 12.00  1.555  1.555  1.555  1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       22 Do !
        C(6)-C(5)-C(22-N(1)   32.00 13.00  1.555  1.555  1.555  1.555
PLAT793_ALERT_4_G The Model has Chirality at C1     (Centro SPGR)       R Verify
PLAT793_ALERT_4_G The Model has Chirality at C3     (Centro SPGR)       S Verify
PLAT882_ALERT_1_G Missing datum for _diffrn_reflns_av_unetI/netI ..... Please Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
 451 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
 444 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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