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: _shoji6

Bond precision: C-C = 0.0032 A   Wavelength=0.71075

Cell: a=11.3188(8)   b=11.0322(8)   c=13.3367(9)
                 alpha=90   beta=92.0346(17)   gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1664.3(2)	1664.3(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
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	1.251	1.251
Z	4	4
Mu (mm-1)	0.076	0.076
F000	664.0	664.0
F000'	664.26	
h,k,lmax	14,14,17	14,14,17
Nref	3802	3784
Tmin,Tmax	0.938,0.970	
Tmin'	0.859	

Correction method= Not given

Data completeness= 0.995   Theta(max)= 27.420

R(reflections)= 0.0699(2430)   wR2(reflections)= 0.1416(2448)

S = 0.951   Npar= 236

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 B

CRYSS02_ALERT_3_B The value of _exptl_crystal_size_max is > 1.0
   Maximum crystal size given =   2.000

🟡 Alert level C

DIFMX01_ALERT_2_C The maximum difference density is > 0.1*ZMAX*0.75
          _refine_diff_density_max given =   0.630
          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.
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density   0.63 eA-3
PLAT193_ALERT_1_C Cell and Diffraction Temperatures Differ by ....   3 Degree
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(3) ...... Senseless s.u.
          C(3) -H(1)   1.555   1.555 ....   #   29 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(3) ...... Senseless s.u.
          C(4) -H(2)   1.555   1.555 ....   #   30 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(4) ...... Senseless s.u.
          C(5) -H(3)   1.555   1.555 ....   #   31 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(4) ...... Senseless s.u.
          C(6) -H(4)   1.555   1.555 ....   #   32 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(3) ...... Senseless s.u.
          C(7) -H(5)   1.555   1.555 ....   #   33 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(3) ...... Senseless s.u.
          C(8) -H(6)   1.555   1.555 ....   #   34 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(3) ...... Senseless s.u.
          C(12)-H(7)   1.555   1.555 ....   #   35 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(3) ...... Senseless s.u.
          C(12)-H(8)   1.555   1.555 ....   #   36 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(3) ...... Senseless s.u.
          C(13)-H(9)   1.555   1.555 ....   #   37 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(3) ...... Senseless s.u.
          C(13)-H(10)   1.555   1.555 ....   #   38 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(3) ...... Senseless s.u.
          C(14)-H(11)   1.555   1.555 ....   #   39 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(3) ...... Senseless s.u.
          C(15)-H(12)   1.555   1.555 ....   #   40 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(3) ...... Senseless s.u.
          C(15)-H(13)   1.555   1.555 ....   #   41 Check
PLAT751_ALERT_4_C Bond   Calc   0.95000, Rep   0.950(2) ...... Senseless s.u.
          C(16)-H(14)   1.555   1.555 ....   #   42 Check
PLAT752_ALERT_4_C Angle   Calc   117.00, Rep   117.5(2) ...... Senseless s.u.
          C(2) -C(3) -H(1)   1.555   1.555   1.555 ....   #   44 Check
PLAT752_ALERT_4_C Angle   Calc   118.00, Rep   118.2(2) ...... Senseless s.u.
          C(4) -C(3) -H(1)   1.555   1.555   1.555 ....   #   45 Check
PLAT752_ALERT_4_C Angle   Calc   118.00, Rep   118.3(3) ...... Senseless s.u.
          C(3) -C(4) -H(2)   1.555   1.555   1.555 ....   #   46 Check
PLAT752_ALERT_4_C Angle   Calc   119.00, Rep   118.9(3) ...... Senseless s.u.
          C(10)-C(4) -H(2)   1.555   1.555   1.555 ....   #   47 Check
PLAT752_ALERT_4_C Angle   Calc   119.00, Rep   119.4(3) ...... Senseless s.u.
          C(6) -C(5) -H(3)   1.555   1.555   1.555 ....   #   48 Check
PLAT752_ALERT_4_C Angle   Calc   119.00, Rep   119.0(3) ...... Senseless s.u.
          C(10)-C(5) -H(3)   1.555   1.555   1.555 ....   #   49 Check
PLAT752_ALERT_4_C Angle   Calc   120.00, Rep   119.9(3) ...... Senseless s.u.
          C(5) -C(6) -H(4)   1.555   1.555   1.555 ....   #   50 Check
PLAT752_ALERT_4_C Angle   Calc   121.00, Rep   120.8(3) ...... Senseless s.u.
          C(7) -C(6) -H(4)   1.555   1.555   1.555 ....   #   51 Check
PLAT752_ALERT_4_C Angle   Calc   119.00, Rep   119.1(3) ...... Senseless s.u.
          C(6) -C(7) -H(5)   1.555   1.555   1.555 ....   #   52 Check
PLAT752_ALERT_4_C Angle   Calc   120.00, Rep   120.3(3) ...... Senseless s.u.
          C(8) -C(7) -H(5)   1.555   1.555   1.555 ....   #   53 Check

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PLAT752_ALERT_4_C Angle   Calc      120.00, Rep     119.9(2) ......   Senseless s.u.
          C(7) -C(8) -H(6)      1.555   1.555   1.555 ....      #   54 Check
PLAT752_ALERT_4_C Angle   Calc      120.00, Rep     119.6(2) ......   Senseless s.u.
          C(9) -C(8) -H(6)      1.555   1.555   1.555 ....      #   55 Check
PLAT752_ALERT_4_C Angle   Calc      111.00, Rep     110.6(2) ......   Senseless s.u.
          O(1) -C(12)-H(7)      1.555   1.555   1.555 ....      #   56 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep     109.6(2) ......   Senseless s.u.
          O(1) -C(12)-H(8)      1.555   1.555   1.555 ....      #   57 Check
PLAT752_ALERT_4_C Angle   Calc      111.00, Rep     110.6(2) ......   Senseless s.u.
          C(2) -C(12)-H(7)      1.555   1.555   1.555 ....      #   58 Check
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep     109.5(2) ......   Senseless s.u.
          C(2) -C(12)-H(8)      1.555   1.555   1.555 ....      #   59 Check
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep     109.5(3) ......   Senseless s.u.
          H(7) -C(12)-H(8)      1.555   1.555   1.555 ....      #   60 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep     110.2(2) ......   Senseless s.u.
          O(1) -C(13)-H(9)      1.555   1.555   1.555 ....      #   61 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep     109.6(2) ......   Senseless s.u.
          O(1) -C(13)-H(10)     1.555   1.555   1.555 ....      #   62 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep     110.4(2) ......   Senseless s.u.
          C(14)-C(13)-H(9)      1.555   1.555   1.555 ....      #   63 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep     110.5(2) ......   Senseless s.u.
          C(14)-C(13)-H(10)     1.555   1.555   1.555 ....      #   64 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep     109.5(3) ......   Senseless s.u.
          H(9) -C(13)-H(10)     1.555   1.555   1.555 ....      #   65 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep     110.0(2) ......   Senseless s.u.
          C(2) -C(14)-H(11)     1.555   1.555   1.555 ....      #   66 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep     110.4(2) ......   Senseless s.u.
          C(13)-C(14)-H(11)     1.555   1.555   1.555 ....      #   67 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep     109.9(2) ......   Senseless s.u.
          C(15)-C(14)-H(11)     1.555   1.555   1.555 ....      #   68 Check
PLAT752_ALERT_4_C Angle   Calc      111.00, Rep     111.0(2) ......   Senseless s.u.
          C(14)-C(15)-H(12)     1.555   1.555   1.555 ....      #   69 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep     110.0(2) ......   Senseless s.u.
          C(14)-C(15)-H(13)     1.555   1.555   1.555 ....      #   70 Check
PLAT752_ALERT_4_C Angle   Calc      111.00, Rep     111.4(2) ......   Senseless s.u.
          C(16)-C(15)-H(12)     1.555   1.555   1.555 ....      #   71 Check
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep     108.9(2) ......   Senseless s.u.
          C(16)-C(15)-H(13)     1.555   1.555   1.555 ....      #   72 Check
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep     109.5(3) ......   Senseless s.u.
          H(12)-C(15)-H(13)     1.555   1.555   1.555 ....      #   73 Check
PLAT752_ALERT_4_C Angle   Calc      107.00, Rep     107.1(2) ......   Senseless s.u.
          C(1) -C(16)-H(14)     1.555   1.555   1.555 ....      #   74 Check
PLAT752_ALERT_4_C Angle   Calc      106.00, Rep     106.0(2) ......   Senseless s.u.
          C(15)-C(16)-H(14)     1.555   1.555   1.555 ....      #   75 Check
PLAT752_ALERT_4_C Angle   Calc      107.00, Rep     107.4(2) ......   Senseless s.u.
          C(17)-C(16)-H(14)     1.555   1.555   1.555 ....      #   76 Check
PLAT754_ALERT_4_C Contact Calc      2.84000, Rep     2.840(2) ......   Senseless s.u.
          O(1) -H(1)        1.555   2.756 ............      #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.49000, Rep     3.487(3) ......   Senseless s.u.
          O(1) -H(2)        1.555   2.756 ............      #   47 Check
PLAT754_ALERT_4_C Contact Calc      2.79000, Rep     2.791(2) ......   Senseless s.u.
          O(1) -H(12)       1.555   4.554 ............      #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.13000, Rep     3.133(3) ......   Senseless s.u.
          N(1) -H(1)        1.555   2.756 ............      #   47 Check
PLAT754_ALERT_4_C Contact Calc      2.76000, Rep     2.760(3) ......   Senseless s.u.
          N(1) -H(4)        1.555   2.656 ............      #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.02000, Rep     3.017(3) ......   Senseless s.u.
          N(1) -H(8)        1.555   2.756 ............      #   47 Check
PLAT754_ALERT_4_C Contact Calc      2.71000, Rep     2.713(3) ......   Senseless s.u.
          N(1) -H(9)        1.555   2.756 ............      #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.45000, Rep     3.446(3) ......   Senseless s.u.
          N(1) -H(11)       1.555   2.756 ............      #   47 Check
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PLAT754_ALERT_4_C Contact Calc    2.90000, Rep   2.901(2) ...... Senseless s.u.
            N(1) -H(14)      1.555   4.554 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.37000, Rep   3.371(3) ...... Senseless s.u.
            C(3) -H(10)      1.555   2.746 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.04000, Rep   3.043(3) ...... Senseless s.u.
            C(3) -H(11)      1.555   3.757 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.40000, Rep   3.397(3) ...... Senseless s.u.
            C(3) -H(12)      1.555   3.757 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.50000, Rep   3.498(3) ...... Senseless s.u.
            C(4) -H(10)      1.555   2.746 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.36000, Rep   3.362(3) ...... Senseless s.u.
            C(4) -H(11)      1.555   3.757 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.26000, Rep   3.259(3) ...... Senseless s.u.
            C(5) -H(6)       1.555   2.646 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.36000, Rep   3.359(4) ...... Senseless s.u.
            C(6) -H(6)       1.555   2.646 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.35000, Rep   3.351(3) ...... Senseless s.u.
            C(6) -H(9)       1.555   1.455 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.58000, Rep   3.581(4) ...... Senseless s.u.
            C(7) -H(3)       1.555   2.656 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.53000, Rep   3.526(3) ...... Senseless s.u.
            C(7) -H(9)       1.555   1.455 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.43000, Rep   3.432(3) ...... Senseless s.u.
            C(8) -H(3)       1.555   2.656 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.54000, Rep   3.535(3) ...... Senseless s.u.
            C(11)-H(4)       1.555   2.656 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.41000, Rep   3.407(3) ...... Senseless s.u.
            C(11)-H(8)       1.555   2.756 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.36000, Rep   3.361(3) ...... Senseless s.u.
            C(12)-H(12)      1.555   4.554 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.38000, Rep   3.375(3) ...... Senseless s.u.
            C(12)-H(13)      1.555   2.746 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.54000, Rep   3.535(3) ...... Senseless s.u.
            C(13)-H(1)       1.555   2.756 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.50000, Rep   3.500(3) ...... Senseless s.u.
            C(13)-H(4)       1.555   1.655 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.40000, Rep   3.404(3) ...... Senseless s.u.
            C(13)-H(5)       1.555   1.655 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.39000, Rep   3.391(3) ...... Senseless s.u.
            C(14)-H(1)       1.555   3.757 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.30000, Rep   3.300(3) ...... Senseless s.u.
            C(15)-H(1)       1.555   3.757 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.59000, Rep   3.586(3) ...... Senseless s.u.
            C(15)-H(7)       1.555   4.555 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.46000, Rep   3.457(3) ...... Senseless s.u.
            C(15)-H(8)       1.555   2.756 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.44000, Rep   3.437(3) ...... Senseless s.u.
            C(16)-H(7)       1.555   4.555 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    2.82000, Rep   2.821(3) ...... Senseless s.u.
            C(17)-H(7)       1.555   4.555 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    2.91000, Rep   2.910(3) ...... Senseless s.u.
            C(18)-H(7)       1.555   4.555 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.26000, Rep   3.259(3) ...... Senseless s.u.
            C(19)-H(7)       1.555   4.555 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.28000, Rep   3.284(4) ...... Senseless s.u.
            C(20)-H(5)       1.555   3.667 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.50000, Rep   3.505(4) ...... Senseless s.u.
            C(20)-H(7)       1.555   4.555 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.41000, Rep   3.411(3) ...... Senseless s.u.
            C(21)-H(2)       1.555   1.565 ............    #   47 Check
PLAT754_ALERT_4_C Contact Calc    3.43000, Rep   3.430(3) ...... Senseless s.u.
            C(21)-H(7)       1.555   4.555 ............    #   47 Check
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PLAT754_ALERT_4_C Contact Calc     3.56000, Rep    3.558(4) ......   Senseless s.u.
             C(21)-H(10)      1.555   3.767 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.37000, Rep    3.370(3) ......   Senseless s.u.
             C(21)-H(12)      1.555   3.767 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.50000, Rep    3.496(3) ......   Senseless s.u.
             C(21)-H(13)      1.555   3.767 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.09000, Rep    3.092(3) ......   Senseless s.u.
             C(22)-H(7)       1.555   4.555 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.31000, Rep    3.307(3) ......   Senseless s.u.
             C(22)-H(8)       1.555   2.756 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.84000, Rep    2.840(2) ......   Senseless s.u.
             H(1) -O(1)       1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.13000, Rep    3.133(3) ......   Senseless s.u.
             H(1) -N(1)       1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.54000, Rep    3.535(3) ......   Senseless s.u.
             H(1) -C(13)      1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.39000, Rep    3.391(3) ......   Senseless s.u.
             H(1) -C(14)      1.555   3.757 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.30000, Rep    3.300(3) ......   Senseless s.u.
             H(1) -C(15)      1.555   3.757 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.16000, Rep    3.161(3) ......   Senseless s.u.
             H(1) -H(10)      1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.69000, Rep    2.685(3) ......   Senseless s.u.
             H(1) -H(11)      1.555   3.757 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.61000, Rep    2.612(3) ......   Senseless s.u.
             H(1) -H(12)      1.555   3.757 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.39000, Rep    3.387(3) ......   Senseless s.u.
             H(1) -H(14)      1.555   3.757 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.49000, Rep    3.487(3) ......   Senseless s.u.
             H(2) -O(1)       1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.41000, Rep    3.411(3) ......   Senseless s.u.
             H(2) -C(21)      1.555   1.545 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.45000, Rep    3.452(3) ......   Senseless s.u.
             H(2) -H(5)       1.555   2.646 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.35000, Rep    3.353(3) ......   Senseless s.u.
             H(2) -H(10)      1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.29000, Rep    3.291(3) ......   Senseless s.u.
             H(2) -H(11)      1.555   3.757 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.26000, Rep    3.263(3) ......   Senseless s.u.
             H(2) -H(12)      1.555   3.757 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.58000, Rep    3.581(4) ......   Senseless s.u.
             H(3) -C(7)       1.555   2.646 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.43000, Rep    3.432(3) ......   Senseless s.u.
             H(3) -C(8)       1.555   2.646 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.17000, Rep    3.170(4) ......   Senseless s.u.
             H(3) -H(5)       1.555   2.646 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.88000, Rep    2.879(3) ......   Senseless s.u.
             H(3) -H(6)       1.555   2.646 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.76000, Rep    2.760(3) ......   Senseless s.u.
             H(4) -N(1)       1.555   2.646 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.54000, Rep    3.535(3) ......   Senseless s.u.
             H(4) -C(11)      1.555   2.646 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.50000, Rep    3.500(3) ......   Senseless s.u.
             H(4) -C(13)      1.555   1.455 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.12000, Rep    3.124(4) ......   Senseless s.u.
             H(4) -H(6)       1.555   2.646 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.63000, Rep    2.633(3) ......   Senseless s.u.
             H(4) -H(9)       1.555   1.455 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.40000, Rep    3.404(3) ......   Senseless s.u.
             H(5) -C(13)      1.555   1.455 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.28000, Rep    3.284(4) ......   Senseless s.u.
             H(5) -C(20)      1.555   3.667 ............   #   47 Check
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PLAT754_ALERT_4_C Contact Calc      3.45000, Rep    3.452(3) ......   Senseless s.u.
            H(5) -H(2)        1.555   2.656 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.17000, Rep    3.170(4) ......   Senseless s.u.
            H(5) -H(3)        1.555   2.656 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      2.97000, Rep    2.970(3) ......   Senseless s.u.
            H(5) -H(9)        1.555   1.455 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      2.96000, Rep    2.957(3) ......   Senseless s.u.
            H(5) -H(10)       1.555   1.455 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.26000, Rep    3.259(3) ......   Senseless s.u.
            H(6) -C(5)        1.555   2.656 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.36000, Rep    3.359(4) ......   Senseless s.u.
            H(6) -C(6)        1.555   2.656 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      2.88000, Rep    2.879(3) ......   Senseless s.u.
            H(6) -H(3)        1.555   2.656 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.12000, Rep    3.124(4) ......   Senseless s.u.
            H(6) -H(4)        1.555   2.656 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.59000, Rep    3.586(3) ......   Senseless s.u.
            H(7) -C(15)       1.555   4.554 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.44000, Rep    3.437(3) ......   Senseless s.u.
            H(7) -C(16)       1.555   4.554 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      2.82000, Rep    2.821(3) ......   Senseless s.u.
            H(7) -C(17)       1.555   4.554 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      2.91000, Rep    2.910(3) ......   Senseless s.u.
            H(7) -C(18)       1.555   4.554 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.26000, Rep    3.259(3) ......   Senseless s.u.
            H(7) -C(19)       1.555   4.554 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.50000, Rep    3.505(4) ......   Senseless s.u.
            H(7) -C(20)       1.555   4.554 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.43000, Rep    3.430(3) ......   Senseless s.u.
            H(7) -C(21)       1.555   4.554 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.09000, Rep    3.092(3) ......   Senseless s.u.
            H(7) -C(22)       1.555   4.554 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.04000, Rep    3.041(3) ......   Senseless s.u.
            H(7) -H(12)       1.555   4.554 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.50000, Rep    3.497(3) ......   Senseless s.u.
            H(7) -H(13)       1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.38000, Rep    3.384(3) ......   Senseless s.u.
            H(7) -H(14)       1.555   4.554 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.02000, Rep    3.017(3) ......   Senseless s.u.
            H(8) -N(1)        1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.41000, Rep    3.407(3) ......   Senseless s.u.
            H(8) -C(11)       1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.46000, Rep    3.457(3) ......   Senseless s.u.
            H(8) -C(15)       1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.31000, Rep    3.307(3) ......   Senseless s.u.
            H(8) -C(22)       1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.22000, Rep    3.225(3) ......   Senseless s.u.
            H(8) -H(10)       1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      2.51000, Rep    2.511(3) ......   Senseless s.u.
            H(8) -H(13)       1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      2.71000, Rep    2.713(3) ......   Senseless s.u.
            H(9) -N(1)        1.555   2.746 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.35000, Rep    3.351(3) ......   Senseless s.u.
            H(9) -C(6)        1.555   1.655 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.53000, Rep    3.526(3) ......   Senseless s.u.
            H(9) -C(7)        1.555   1.655 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      2.63000, Rep    2.633(3) ......   Senseless s.u.
            H(9) -H(4)        1.555   1.655 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      2.97000, Rep    2.970(3) ......   Senseless s.u.
            H(9) -H(5)        1.555   1.655 ............   #   47 Check
PLAT754_ALERT_4_C Contact Calc      3.37000, Rep    3.371(3) ......   Senseless s.u.
            H(10)-C(3)        1.555   2.756 ............   #   47 Check
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PLAT754_ALERT_4_C Contact Calc     3.50000, Rep    3.498(3) ...... Senseless s.u.
            H(10)-C(4)        1.555   2.756 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.56000, Rep    3.558(4) ...... Senseless s.u.
            H(10)-C(21)       1.555   3.767 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.16000, Rep    3.161(3) ...... Senseless s.u.
            H(10)-H(1)        1.555   2.756 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.35000, Rep    3.353(3) ...... Senseless s.u.
            H(10)-H(2)        1.555   2.756 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.96000, Rep    2.957(3) ...... Senseless s.u.
            H(10)-H(5)        1.555   1.655 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.22000, Rep    3.225(3) ...... Senseless s.u.
            H(10)-H(8)        1.555   2.756 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.45000, Rep    3.446(3) ...... Senseless s.u.
            H(11)-N(1)        1.555   2.746 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.04000, Rep    3.043(3) ...... Senseless s.u.
            H(11)-C(3)        1.555   3.757 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.36000, Rep    3.362(3) ...... Senseless s.u.
            H(11)-C(4)        1.555   3.757 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.69000, Rep    2.685(3) ...... Senseless s.u.
            H(11)-H(1)        1.555   3.757 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.29000, Rep    3.291(3) ...... Senseless s.u.
            H(11)-H(2)        1.555   3.757 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.95000, Rep    2.946(3) ...... Senseless s.u.
            H(11)-H(11)       1.555   3.757 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.43000, Rep    3.433(3) ...... Senseless s.u.
            H(11)-H(14)       1.555   3.757 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.79000, Rep    2.791(2) ...... Senseless s.u.
            H(12)-O(1)        1.555   4.555 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.40000, Rep    3.397(3) ...... Senseless s.u.
            H(12)-C(3)        1.555   3.757 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.36000, Rep    3.361(3) ...... Senseless s.u.
            H(12)-C(12)       1.555   4.555 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.37000, Rep    3.370(3) ...... Senseless s.u.
            H(12)-C(21)       1.555   3.767 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.61000, Rep    2.612(3) ...... Senseless s.u.
            H(12)-H(1)        1.555   3.757 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.26000, Rep    3.263(3) ...... Senseless s.u.
            H(12)-H(2)        1.555   3.757 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.04000, Rep    3.041(3) ...... Senseless s.u.
            H(12)-H(7)        1.555   4.555 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.38000, Rep    3.375(3) ...... Senseless s.u.
            H(13)-C(12)       1.555   2.756 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.50000, Rep    3.496(3) ...... Senseless s.u.
            H(13)-C(21)       1.555   3.767 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.50000, Rep    3.497(3) ...... Senseless s.u.
            H(13)-H(7)        1.555   2.756 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.51000, Rep    2.511(3) ...... Senseless s.u.
            H(13)-H(8)        1.555   2.756 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     2.90000, Rep    2.901(2) ...... Senseless s.u.
            H(14)-N(1)        1.555   4.555 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.39000, Rep    3.387(3) ...... Senseless s.u.
            H(14)-H(1)        1.555   3.757 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.38000, Rep    3.384(3) ...... Senseless s.u.
            H(14)-H(7)        1.555   4.555 .............    #   47 Check
PLAT754_ALERT_4_C Contact Calc     3.43000, Rep    3.433(3) ...... Senseless s.u.
            H(14)-H(11)       1.555   3.757 .............    #   47 Check
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⬤ Alert level G

CHEMS02_ALERT_1_G Please check that you have entered the correct
        _publ_requested_category classification of your compound;

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                    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 ....        2.00 mm
PLAT200_ALERT_1_G Reported    _diffrn_ambient_temperature ..... (K)        293 Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C1       -- C11      ..       6.8 s.u.
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          8 Do !
              C(2)-C(1)-C(11-N(1)  127.00 11.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         17 Do !
              C(9)-C(1)-C(11-N(1)    0.00 11.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         26 Do !
              C(16-C(1)-C(11-N(1) -122.00 11.00   1.555   1.555   1.555   1.555
PLAT793_ALERT_4_G The Model has Chirality at C1       (Centro SPGR)         S Verify
PLAT793_ALERT_4_G The Model has Chirality at C2       (Centro SPGR)         S Verify
PLAT793_ALERT_4_G The Model has Chirality at C14      (Centro SPGR)         S Verify
PLAT793_ALERT_4_G The Model has Chirality at C16      (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
   1 ALERT level B = A potentially serious problem, consider carefully
 180 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
 184 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

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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