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: 3166

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Bond precision:   C-C = 0.0882 A          Wavelength=0.71073

Cell:         a=13.4104(15)       b=13.4700(15)    c=13.8314(14)
              alpha=118.487(11)   beta=94.653(9)   gamma=95.911(9)
Temperature:  293 K

                  Calculated                Reported
Volume            2159.9(5)                 2159.9(5)
Space group       P -1                      P -1
Hall group        -P 1                      -P 1
Moiety formula    C46 H110 K4 Li6 O10 Si6,  C46 H110 K4 Li8 O10 Si6,
                  2(C4 H8 O), 2(Li)         2(C4 H8 O)
Sum formula       C54 H126 K4 Li8 O12 Si6   C54 H132 K4 Li8 O12 Si6
Mr                1348.01                   1354.05
Dx,g cm-3         1.036                     1.041
Z                 1                         1
Mu (mm-1)         0.332                     0.332
F000              730.0                     736.0
F000'             731.52
h,k,lmax          18,18,18                  18,18,17
Nref              11722                     9720
Tmin,Tmax         0.911,0.920               0.926,1.000
Tmin'             0.911

Correction method= # Reported T Limits: Tmin=0.926 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.829         Theta(max)= 29.204

R(reflections)= 0.4184( 3462)     wR2(reflections)= 0.7891( 9720)

S = 2.945                  Npar= 390
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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.

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🔴 **Alert level A**

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
            Absolute value of the parameter shift to su ratio given   2.945
            Additional refinement cycles may be required.
PLAT080_ALERT_2_A Maximum Shift/Error ....   2.94 Why ?
PLAT082_ALERT_2_A High R1 Value ....   0.42 Report
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ....   0.79 Report
PLAT094_ALERT_2_A Ratio of Maximum / Minimum Residual Density ....   9.22 Report
PLAT097_ALERT_2_A Large Reported Max. (Positive) Residual Density   10.84 eA-3
PLAT211_ALERT_2_A ADP of Atom Li11   is N.P.D. or (nearly) 2D .   Please Check
PLAT211_ALERT_2_A ADP of Atom Li12   is N.P.D. or (nearly) 2D .   Please Check
PLAT213_ALERT_2_A Atom O5   has ADP max/min Ratio .....   5.8 prolat
PLAT213_ALERT_2_A Atom C00L   has ADP max/min Ratio .....   7.9 prolat
PLAT213_ALERT_2_A Atom C00N   has ADP max/min Ratio .....   8.6 prolat
PLAT213_ALERT_2_A Atom C00W   has ADP max/min Ratio .....   5.9 prolat
PLAT214_ALERT_2_A Atom C01A   (Anion/Solvent) ADP max/min Ratio   12.8 prolat
PLAT234_ALERT_4_A Large Hirshfeld Difference Si2   --C00N   0.39 Ang.
PLAT234_ALERT_4_A Large Hirshfeld Difference Si2   --C00T   0.44 Ang.
PLAT234_ALERT_4_A Large Hirshfeld Difference C00V   --C014   0.49 Ang.
PLAT234_ALERT_4_A Large Hirshfeld Difference C010   --C014   0.45 Ang.
PLAT340_ALERT_3_A Low Bond Precision on C-C Bonds ....   0.08818 Ang.
PLAT351_ALERT_3_A Long   C-H (X0.96,N1.08A) C15   - H16A   ..   1.40 Ang.
PLAT351_ALERT_3_A Long   C-H (X0.96,N1.08A) C15   - H16B   ..   1.40 Ang.
PLAT360_ALERT_2_A Short   C(sp3)-C(sp3) Bond C00K   - C00W   .   1.10 Ang.
PLAT360_ALERT_2_A Short   C(sp3)-C(sp3) Bond C013   - C01A   .   1.19 Ang.

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🟠 **Alert level B**

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low ..   36% Check
PLAT212_ALERT_2_B ADP of Atom Li17   is N.P.D. or (nearly) 2D .   Please Check
PLAT213_ALERT_2_B Atom C00J   has ADP max/min Ratio .....   4.7 prolat
PLAT213_ALERT_2_B Atom C010   has ADP max/min Ratio .....   4.5 prolat
PLAT234_ALERT_4_B Large Hirshfeld Difference Si1   --C00I   0.30 Ang.
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of   Li12 Check
PLAT242_ALERT_2_B Low   'MainMol' Ueq as Compared to Neighbors of   Si00 Check
PLAT242_ALERT_2_B Low   'MainMol' Ueq as Compared to Neighbors of   Si2 Check
PLAT360_ALERT_2_B Short   C(sp3)-C(sp3) Bond C00X   - C00Z   .   1.27 Ang.
PLAT366_ALERT_2_B Short? C(sp?)-C(sp?) Bond C15   - C16   .   0.93 Ang.
PLAT412_ALERT_2_B Short Intra XH3 .. XHn   H00I   ..Hk   1.78 Ang.
PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set   Please Do !

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🟡 **Alert level C**

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
            The relevant atom site should be identified.
GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
            outside the range 0.80 <> 2.00
            Goodness of fit given =   2.945
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..   6.04 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT087_ALERT_2_C Unsatisfactory S value (Too High) ....   2.94 Check
PLAT213_ALERT_2_C Atom O0C   has ADP max/min Ratio .....   3.4 prolat
PLAT213_ALERT_2_C Atom C00O   has ADP max/min Ratio .....   3.1 oblate
PLAT213_ALERT_2_C Atom C00R   has ADP max/min Ratio .....   4.0 prolat
PLAT213_ALERT_2_C Atom C00U   has ADP max/min Ratio .....   3.1 prolat

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PLAT213_ALERT_2_C Atom C16              has ADP max/min Ratio .....      3.7 prolat
PLAT213_ALERT_2_C Atom C00Y             has ADP max/min Ratio .....      3.1 prolat
PLAT213_ALERT_2_C Atom Li15             has ADP max/min Ratio .....      3.1 prolat
PLAT220_ALERT_2_C Non-Solvent  Resd 1 C   Ueq(max)/Ueq(min) Range       3.2 Ratio
PLAT220_ALERT_2_C Non-Solvent  Resd 1 Li  Ueq(max)/Ueq(min) Range       3.1 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range      4.2 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O5 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C00V Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C00Y Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     K002 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      Si1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C00H Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C00K Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     C00Z Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     Li11 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of     C01A Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of     C013 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of     C0AA Check
PLAT303_ALERT_2_C Full Occupancy Atom H16A      with # Connections     2.00 Check
PLAT303_ALERT_2_C Full Occupancy Atom H16B      with # Connections     2.00 Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C00H    - C00L    .        1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C00V    - C014    .        1.42 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C00S    - C00Y    ..       1.68 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C00Y    - C00Z    ..       1.65 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H01B    ..H01B             2.13 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H00J    ..Hj               1.83 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H00L    ..H00U             1.84 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H00D    ..H01A             2.11 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H00Z    ..H00Z             2.10 Ang.
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🔘 **Alert level G**

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C54 H132 K4 Li8 O12 Si6
           Atom count from _chemical_formula_moiety:C54 H126 K4 Li8 O12 Si6
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C54 H132 K4 Li8 O12 Si6
           Atom count from the _atom_site data:  C54 H126 K4 Li8 O12 Si6
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
           From the CIF: _cell_formula_units_Z    1
           From the CIF: _chemical_formula_sum  C54 H132 K4 Li8 O12 Si6
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         54.00     54.00    0.00
           H        132.00    126.00    6.00
           K          4.00      4.00    0.00
           Li         8.00      8.00    0.00
           O         12.00     12.00    0.00
           Si         6.00      6.00    0.00
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......   Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ   Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large     0.15 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)      293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)       293 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for     C00H Check
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PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for     C00K Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C00O Check
PLAT343_ALERT_2_G Unusual         Angle Range in Main Residue for      C15 Check
PLAT343_ALERT_2_G Unusual sp3     Angle Range in Main Residue for       C16 Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range in Main Residue for      C010 Check
PLAT344_ALERT_2_G Unusual sp?      Angle Range in Solvent/Ion for       C14 Check
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond  C14      - C013      .      1.75 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      89 Note
PLAT721_ALERT_1_G Bond   Calc    0.95000, Rep    0.96100 Dev...     0.01 Ang.
          C00I     -H00D          1.555   1.555 ........     #  50 Check
PLAT721_ALERT_1_G Bond   Calc    0.95000, Rep    0.96030 Dev...     0.01 Ang.
          C00N     -H00S          1.555   1.555 ........     #  67 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    1.01530 Dev...     0.05 Ang.
          C00Q     -H00Y          1.555   1.555 ........     #  75 Check
PLAT721_ALERT_1_G Bond   Calc    0.96000, Rep    1.01630 Dev...     0.06 Ang.
          C00Q     -H             1.555   1.555 ........     #  76 Check
PLAT721_ALERT_1_G Bond   Calc    0.96000, Rep    1.02100 Dev...     0.06 Ang.
          C00Q     -HA            1.555   1.555 ........     #  77 Check
PLAT721_ALERT_1_G Bond   Calc    0.96000, Rep    1.02410 Dev...     0.06 Ang.
          C00R     -H00Z          1.555   1.555 ........     #  78 Check
PLAT721_ALERT_1_G Bond   Calc    0.96000, Rep    1.02230 Dev...     0.06 Ang.
          C00R     -HB            1.555   1.555 ........     #  79 Check
PLAT721_ALERT_1_G Bond   Calc    0.96000, Rep    1.02300 Dev...     0.06 Ang.
          C00R     -HC            1.555   1.555 ........     #  80 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    1.08550 Dev...     0.12 Ang.
          C00T     -H0AA          1.555   1.555 ........     #  84 Check
PLAT721_ALERT_1_G Bond   Calc    0.96000, Rep    1.07150 Dev...     0.11 Ang.
          C00T     -HE            1.555   1.555 ........     #  85 Check
PLAT721_ALERT_1_G Bond   Calc    0.95000, Rep    1.08320 Dev...     0.13 Ang.
          C00T     -HF            1.555   1.555 ........     #  86 Check
PLAT721_ALERT_1_G Bond   Calc    0.97000, Rep    0.96000 Dev...     0.01 Ang.
          C00U     -HH            1.555   1.555 ........     #  89 Check
PLAT721_ALERT_1_G Bond   Calc    0.96000, Rep    0.97000 Dev...     0.01 Ang.
          C00Y     -H5AA          1.555   1.555 ........     #  99 Check
PLAT721_ALERT_1_G Bond   Calc    0.96000, Rep    0.97000 Dev...     0.01 Ang.
          C014     -H01C          1.555   1.555 ........     # 125 Check
PLAT721_ALERT_1_G Bond   Calc    0.96000, Rep    0.97000 Dev...     0.01 Ang.
          C01A     -H01H          1.555   1.555 ........     # 136 Check
PLAT721_ALERT_1_G Bond   Calc    0.96000, Rep    0.97000 Dev...     0.01 Ang.
          C14      -H14A          1.555   1.555 ........     # 139 Check
PLAT721_ALERT_1_G Bond   Calc    0.96000, Rep    0.97000 Dev...     0.01 Ang.
          C0AA     -H0AC          1.555   1.555 ........     # 142 Check
PLAT721_ALERT_1_G Bond   Calc    0.96000, Rep    0.97000 Dev...     0.01 Ang.
          C16      -H16B          1.555   1.555 ........     # 145 Check
PLAT722_ALERT_1_G Angle  Calc    109.00, Rep    110.20 Dev...     1.20 Degree
          SI1      -C00I    -H00D      1.555  1.555  1.555  # 147 Check
PLAT722_ALERT_1_G Angle  Calc    104.00, Rep    102.80 Dev...     1.20 Degree
          C00W     -C00K    -H00J      1.555  1.555  1.555  # 160 Check
PLAT722_ALERT_1_G Angle  Calc    109.00, Rep    110.30 Dev...     1.30 Degree
          C00H     -C00L    -H00L      1.555  1.555  1.555  # 165 Check
PLAT722_ALERT_1_G Angle  Calc    110.00, Rep    108.30 Dev...     1.70 Degree
          C00H     -C00L    -H00M      1.555  1.555  1.555  # 166 Check
PLAT722_ALERT_1_G Angle  Calc    109.00, Rep    111.10 Dev...     2.10 Degree
          SI2      -C00N    -H00Q      1.555  1.555  1.555  # 176 Check
PLAT722_ALERT_1_G Angle  Calc    110.00, Rep    108.40 Dev...     1.60 Degree
          SI2      -C00N    -H00S      1.555  1.555  1.555  # 178 Check
PLAT722_ALERT_1_G Angle  Calc    113.00, Rep    111.20 Dev...     1.80 Degree
          O00E     -C00O    -H00T      1.555  1.555  1.555  # 182 Check
PLAT722_ALERT_1_G Angle  Calc    111.00, Rep    112.50 Dev...     1.50 Degree
          C010     -C00O    -H00T      1.555  1.555  1.555  # 186 Check
PLAT722_ALERT_1_G Angle  Calc    109.00, Rep    114.00 Dev...     5.00 Degree
          SI1      -C00Q    -H00Y      1.555  1.555  1.555  # 198 Check
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PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      114.30 Dev...      4.30 Degree
         SI1     -C00Q    -H          1.555  1.555  1.555     #  199 Check
PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      115.20 Dev...      5.20 Degree
         SI1     -C00Q    -HA         1.555  1.555  1.555     #  200 Check
PLAT722_ALERT_1_G Angle   Calc     109.00, Rep      104.10 Dev...      4.90 Degree
         H00Y    -C00Q    -H          1.555  1.555  1.555     #  201 Check
PLAT722_ALERT_1_G Angle   Calc     109.00, Rep      104.10 Dev...      4.90 Degree
         H00Y    -C00Q    -HA         1.555  1.555  1.555     #  202 Check
PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      103.80 Dev...      6.20 Degree
         H       -C00Q    -HA         1.555  1.555  1.555     #  203 Check
PLAT722_ALERT_1_G Angle   Calc     109.00, Rep      114.00 Dev...      5.00 Degree
         SI00    -C00R    -H00Z       1.555  1.555  1.555     #  204 Check
PLAT722_ALERT_1_G Angle   Calc     109.00, Rep      113.70 Dev...      4.70 Degree
         SI00    -C00R    -HB         1.555  1.555  1.555     #  205 Check
PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      113.90 Dev...      3.90 Degree
         SI00    -C00R    -HC         1.555  1.555  1.555     #  206 Check
PLAT722_ALERT_1_G Angle   Calc     109.00, Rep      104.80 Dev...      4.20 Degree
         H00Z    -C00R    -HB         1.555  1.555  1.555     #  207 Check
PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      104.70 Dev...      5.30 Degree
         H00Z    -C00R    -HC         1.555  1.555  1.555     #  208 Check
PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      104.70 Dev...      5.30 Degree
         HB      -C00R    -HC         1.555  1.555  1.555     #  209 Check
PLAT722_ALERT_1_G Angle   Calc     111.00, Rep      109.70 Dev...      1.30 Degree
         O00F    -C00S    -HD         1.555  1.555  1.555     #  211 Check
PLAT722_ALERT_1_G Angle   Calc     109.00, Rep      118.20 Dev...      9.20 Degree
         SI2     -C00T    -H0AA       1.555  1.555  1.555     #  216 Check
PLAT722_ALERT_1_G Angle   Calc     109.00, Rep      116.70 Dev...      7.70 Degree
         SI2     -C00T    -HE         1.555  1.555  1.555     #  217 Check
PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      117.90 Dev...      7.90 Degree
         SI2     -C00T    -HF         1.555  1.555  1.555     #  218 Check
PLAT722_ALERT_1_G Angle   Calc     109.00, Rep      100.30 Dev...      8.70 Degree
         H0AA    -C00T    -HE         1.555  1.555  1.555     #  219 Check
PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      100.00 Dev...     10.00 Degree
         H0AA    -C00T    -HF         1.555  1.555  1.555     #  220 Check
PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      100.50 Dev...      9.50 Degree
         HE      -C00T    -HF         1.555  1.555  1.555     #  221 Check
PLAT722_ALERT_1_G Angle   Calc     106.00, Rep      108.00 Dev...      2.00 Degree
         C014    -C00V    -H2AA       1.555  1.555  1.555     #  232 Check
PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      108.00 Dev...      2.00 Degree
         C00K    -C00W    -H3AA       1.555  1.555  1.555     #  234 Check
PLAT722_ALERT_1_G Angle   Calc     111.00, Rep      109.20 Dev...      1.80 Degree
         C00Z    -C00X    -HL         1.555  1.555  1.555     #  245 Check
PLAT722_ALERT_1_G Angle   Calc     113.00, Rep      111.70 Dev...      1.30 Degree
         C00S    -C00Y    -H5AA       1.555  1.555  1.555     #  246 Check
PLAT722_ALERT_1_G Angle   Calc     112.00, Rep      113.10 Dev...      1.10 Degree
         C00Z    -C00Y    -H5AA       1.555  1.555  1.555     #  250 Check
PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      111.60 Dev...      1.60 Degree
         C00X    -C00Z    -H6AA       1.555  1.555  1.555     #  253 Check
PLAT722_ALERT_1_G Angle   Calc     111.00, Rep      109.40 Dev...      1.60 Degree
         C00Y    -C00Z    -HN         1.555  1.555  1.555     #  256 Check
PLAT722_ALERT_1_G Angle   Calc     109.00, Rep      110.30 Dev...      1.30 Degree
         C014    -C010    -H01A       1.555  1.555  1.555     #  262 Check
PLAT722_ALERT_1_G Angle   Calc     112.00, Rep      108.80 Dev...      3.20 Degree
         C01A    -C013    -H01E       1.555  1.555  1.555     #  355 Check
PLAT722_ALERT_1_G Angle   Calc     112.00, Rep      114.90 Dev...      2.90 Degree
         C01A    -C013    -H01F       1.555  1.555  1.555     #  356 Check
PLAT722_ALERT_1_G Angle   Calc     111.00, Rep      112.20 Dev...      1.20 Degree
         C14     -C013    -H01F       1.555  1.555  1.555     #  359 Check
PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      112.20 Dev...      2.20 Degree
         C00V    -C014    -H01D       1.555  1.555  1.555     #  361 Check
PLAT722_ALERT_1_G Angle   Calc     110.00, Rep      106.10 Dev...      3.90 Degree
         C013    -C01A    -H01G       1.555  1.555  1.555     #  417 Check
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PLAT722_ALERT_1_G Angle   Calc        112.00, Rep      116.30 Dev...        4.30 Degree
            C013    -C01A   -H01H      1.555  1.555  1.555    #  418 Check
PLAT722_ALERT_1_G Angle   Calc        114.00, Rep      115.80 Dev...        1.80 Degree
            C013    -C14    -H14A      1.555  1.555  1.555    #  442 Check
PLAT722_ALERT_1_G Angle   Calc        113.00, Rep      110.80 Dev...        2.20 Degree
            C013    -C14    -H14B      1.555  1.555  1.555    #  443 Check
PLAT722_ALERT_1_G Angle   Calc        109.00, Rep      107.10 Dev...        1.90 Degree
            O00G    -C0AA   -H0AC      1.555  1.555  1.555    #  447 Check
PLAT722_ALERT_1_G Angle   Calc         86.00, Rep       83.10 Dev...        2.90 Degree
            K003    -C16    -H16B      2.666  1.555  1.555    #  452 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.84 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C00O      --C010           1.78 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C013      --C14            1.74 Ang.
```

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  22 ALERT level A = Most likely a serious problem - resolve or explain
  12 ALERT level B = A potentially serious problem, consider carefully
  40 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  84 ALERT level G = General information/check it is not something unexpected

  75 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  67 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  10 ALERT type 4 Improvement, methodology, query or suggestion
   0 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.

PLATON version of 23/04/2018; check.def file version of 23/04/2018