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: kennygayite

```
Bond precision:   S- O = 0.0100 A          Wavelength=0.71075

Cell:           a=6.3785(5)        b=7.4519(6)       c=10.3112(8)
                alpha=75.234(5)    beta=79.388(6)    gamma=88.175(6)
Temperature:    293 K

                Calculated                 Reported
Volume          465.76(7)                  465.76(6)
Space group     P -1                       P -1
Hall group      -P 1                       -P 1
Moiety formula  O8 Pb4 S                   ?
Sum formula     O8 Pb4 S                   H2 O8 Pb4 S
Mr              988.86                     990.84
Dx,g cm-3       7.051                      7.065
Z               2                          2
Mu (mm-1)       72.308                     72.310
F000            816.0                      820.0
F000'           793.02
h,k,lmax        9,10,14                    9,10,14
Nref            2841                       2818
Tmin,Tmax       0.002,0.055                0.377,1.000
Tmin'           0.001

Correction method= # Reported T Limits: Tmin=0.377 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992           Theta(max)= 30.502

R(reflections)= 0.0463( 2419)                wR2(reflections)=
                                             0.1187( 2818)
S = 1.057                  Npar= 118
```

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

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.139
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       1.98 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.17 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       7.00 eA-3
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of          S Check
```

Alert level G

```
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:H2 O8 Pb4 S1
           Atom count from the _atom_site data:  O8 Pb4 S1
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    2
          From the CIF: _chemical_formula_sum  H2 O8 Pb4 S
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          H          4.00      0.00    4.00
          O         16.00     16.00    0.00
          Pb         8.00      8.00    0.00
          S          2.00      2.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.139 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       5.53 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          2 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          4 Note
```

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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
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   9 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
   2 ALERT type 3 Indicator that the structure quality may be low
   1 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.

PLATON version of 19/02/2022; check.def file version of 19/02/2022

Datablock kennygayite - ellipsoid plot