# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 250501a_0m_a

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: 250501a_0m_a

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Bond precision:    C-C = 0.0076 A              Wavelength=0.71073

Cell:           a=11.0048(4)        b=12.0426(6)        c=33.1989(17)
                alpha=82.180(2)     beta=87.994(2)      gamma=66.680(2)
Temperature:    173 K
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|  | Calculated | Reported |
|---|---|---|
| Volume | 4001.9(3) | 4001.9(3) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C28 H64 Ge K O6 Si4, C28 H62.71 Ge K O6 Si4 | ? |
| Sum formula | C56 H126.71 Ge2 K2 O12 Si8 | C9.33 H21.12 Ge0.33 K0.33 O2 Si1.33 |
| Mr | 1440.42 | 240.06 |
| Dx,g cm-3 | 1.195 | 1.195 |
| Z | 2 | 12 |
| Mu (mm-1) | 1.022 | 1.022 |
| F000 | 1545.4 | 1545.0 |
| F000' | 1548.56 | |
| h,k,lmax | 13,15,41 | 13,15,41 |
| Nref | 16356 | 16327 |
| Tmin,Tmax | 0.885,0.903 | 0.750,0.862 |
| Tmin' | 0.815 | |

Correction method= # Reported T Limits: Tmin=0.750 Tmax=0.862
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.380

R(reflections)= 0.0591( 11538)

wR2(reflections)=
0.1602( 16327)

S = 1.074                    Npar= 909

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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 C**
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
          a literature citation. This should be contained in the
          _exptl_absorpt_process_details field.
          Absorption correction given as Multi-Scan
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
          Calc: C56 H126.71 Ge2 K2 O12 Si8
          Rep.: C9.33 H21.12 Ge0.33 K0.33 O2 Si1.33
PLAT213_ALERT_2_C Atom C21            has ADP max/min Ratio .....        3.4 prolat
PLAT213_ALERT_2_C Atom C22            has ADP max/min Ratio .....        3.8 prolat
PLAT220_ALERT_2_C NonSolvent    Resd 1  C   Ueq(max)/Ueq(min) Range       4.6 Ratio
PLAT220_ALERT_2_C NonSolvent    Resd 2  C   Ueq(max)/Ueq(min) Range       5.0 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2  H   Uiso(max)/Uiso(min) Range       5.0 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O5      --C41      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C39     --C40      .       0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C38 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C40 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C41 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      K1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     Si2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     Si4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     Si5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     Si6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     Si7 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     Si8 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00758 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.933 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         6 Report
          0 -1  1,   0  1  2,   0  1  3,   0  0  4,   0  0 13, -11 -2 18,
PLAT977_ALERT_2_C Check Negative Difference Density on H46B     .       -0.31 eA-3

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⚪ **Alert level G**
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
          From the CIF: _cell_formula_units_Z   12
          From the CIF: _chemical_formula_sum  C9.33 H21.12 Ge0.33 K0.33 O2 Si1.3
          TEST: Compare cell contents of formula and atom_site data

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           atom    Z*formula  cif sites diff
           C        111.96    112.00   -0.04
           H        253.44    253.42    0.02
           Ge         3.96      4.00   -0.04
           K          3.96      4.00   -0.04
           O         24.00     24.00    0.00
           Si        15.96     16.00   -0.04
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms         36 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.167 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.002 Degree
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         2 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0050 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0050 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par    0.0050 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par    0.0050 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    2)       45% Note
PLAT413_ALERT_2_G Short Inter XH3 .. XHn      H21B    ..H56C      .     2.02 Ang.
                                          -1+x,y,z  =      1_455 Check
PLAT780_ALERT_1_G Coordinates do not Form a Properly Connected Set   Please Do !
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      732 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..   Please Do !
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]=     1.88 Note
           0  1  0,   0  0  1,   0  0  2,   0  0  3,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        18 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        2 Note
           0 -1  1,   0  0  4,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........    2.037 Note
           Predicted wR2: Based on SigI**2  7.87 or SHELX Weight 14.92
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        0 Info
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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
  23 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  23 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  19 ALERT type 2 Indicator that the structure model may be wrong or deficient
  11 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   2 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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**PLATON version of 26/09/2025; check.def file version of 20/09/2025**

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# duplicate check

## No duplication found

**Datablock 250501a_0m_a** - ellipsoid plot