checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 260112lu_zy_1226_0m

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: 260112lu_zy_1226_0m

Bond precision: C-C = 0.0301 A Wavelength=1.34139

Cell: a=41.342(3) b=26.2378(19) c=43.027(3)
alpha=90 beta=108.975(2) gamma=90
Temperature: 223 K

	Calculated	Reported
Volume	44136(5)	44135(5)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C294 H294 Au103 S43 [+ solvent]	C294 H294 Au103 S43
Sum formula	C294 H294 Au103 S43 [+ solvent]	C294 H294 Au103 S43
Mr	25493.65	25493.41
Dx,g cm-3	3.837	3.837
Z	4	4
Mu (mm-1)	44.406	44.697
F000	43532.0	43532.0
F000'	41551.99	
h,k,lmax	49,31,51	49,31,51
Nref	39629	39379
Tmin,Tmax	0.007,0.028	0.225,0.751
Tmin'	0.001	

Correction method= # Reported T Limits: Tmin=0.225 Tmax=0.751
AbsCorr = NONE

Data completeness= 0.994 Theta(max)= 53.378

R(reflections)= 0.1030(23408) wR2(reflections)= 0.3299(39379)

S = 1.152 Npar= 2144

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 A

PLAT057_ALERT_3_A Correction for Absorption Required RT(exp) ... 3.74 Do !

Author Response: All data sets were measured with several scans to increase the number of redundant reflections. In our experience this method of averaging redundant reflections replaces in a good approximation semi-empirical absorptions methods (absorption correction programs like SORTAV lead to no better datasets).

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.96Ang From Au17 7.65 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.93Ang From Au16 7.65 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.04Ang From Au14 7.55 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.03Ang From Au40 7.44 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.10Ang From Au52 7.44 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.13Ang From Au18 7.07 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.03Ang From Au19 6.88 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.03Ang From Au33 6.69 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.98Ang From Au20 6.65 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.97Ang From Au35 6.63 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.00Ang From Au15 6.46 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.10Ang From Au39 6.37 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.14Ang From Au29 6.29 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.11Ang From Au34 6.29 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.05Ang From Au44 6.26 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.04Ang From Au12 6.25 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.20Ang From S4 6.22 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.92Ang From Au11 6.20 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.94Ang From Au10 6.18 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.93Ang From Au8 6.13 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.02Ang From Au6 6.10 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.03Ang From Au37 5.96 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.02Ang From Au33 5.95 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.05Ang From Au30 5.89 eA-3

Author Response: Due to the large metal core of this cluster, the relatively large residual density is close to Au atom, which might be caused by the electronic polarization of the corresponding Au atom.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.97Ang From Au52 -6.08 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.87Ang From Au19 -5.93 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.02Ang From Au29 -5.83 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.73Ang From Au34 -5.54 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.85Ang From Au18 -5.53 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.82Ang From Au17 -5.52 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.74Ang From Au33 -5.48 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.85Ang From Au29 -5.34 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 1.01Ang From Au17 -5.25 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.96Ang From Au32 -5.17 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.91Ang From Au42 -5.16 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.89Ang From Au6 -5.12 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.78Ang From Au18 -5.09 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.97Ang From Au8 -5.08 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.85Ang From Au37 -5.07 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.87Ang From Au34 -5.06 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.99Ang From Au9 -5.05 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.87Ang From Au32 -5.05 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.82Ang From Au8 -5.02 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.84Ang From Au42 -5.02 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.91Ang From Au42 -5.01 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.82Ang From Au40 -4.99 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.88Ang From Au34 -4.98 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.83Ang From Au11 -4.95 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.85Ang From Au19 -4.88 eA-3

Author Response: Beacse of the large metal core of the cluster, thermal vibrations during testing would lead to the presence of residual density around the Au atoms.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Au33 6.14 eA-3

Author Response: The Au atom is a heavy atom and this alert is often found for the large metal core of the cluster.

Alert level B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.03014 Ang.

Author Response: The carbon atoms of C-C bonds in the structure don't have large disorder. Considering the relatively large R(int) of the dataset, the alert is most likely caused by poor data quality.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.120
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.33 Report
PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours S1_16 Check
PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours S1_20 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Au1 0.105 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -8.221 Report

```
PLAT910_ALERT_3_C Missing FCF Reflection(s) Below Theta(Min)[Deg]=       2.81 Note
                1  1  0,   2  0  0,  -1  1  1,   1  1  1,  -2  0  2,  -1  1  2,
                0  0  2,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.598        241 Report
                4  0  0,  36 20  0, -47  1  1, -35 21  1, -14 30  1,   2  2  1,
               38 18  1,  39 17  1,  44 10  1,  46  4  1,  46  2  2, -47  5  3,
              -29 25  3,  14 18  3,  20 28  3, -22 28  4,  -8  0  4, -48  2  5,
              -33 23  5, -25 27  5,  43  9  5, -25 27  6,  38 16  6, -46 10  7,
              -41 17  7,  18 28  7,  29 23  7,  44  2  7, -42 16  8, -41 17  8,
                   (  211 More NOT listed: see .ckf listing file)
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          6 Note
                1  1  0,   2  0  0,  -1  1  1,   1  1  1,  -2  0  2,   0  0  2,
PLAT977_ALERT_2_C Check Negative Difference Density on H7B_1     .      -0.72 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3_2      .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H5_3      .      -0.68 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7B_3     .      -0.58 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2_4      .      -0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3_4      .      -0.40 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6_4      .      -0.77 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6_5      .      -0.47 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H5_7      .      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7B_7     .      -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3_8      .      -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6_8      .      -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6_9      .      -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2_10     .      -0.45 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H5_10     .      -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2_11     .      -0.41 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7A_11    .      -0.55 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6_12     .      -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7C_12    .      -0.41 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7A_13    .      -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7C_13    .      -0.83 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2_14     .      -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7A_14    .      -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3_16     .      -0.60 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H5_16     .      -0.61 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7C_16    .      -0.59 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2_17     .      -0.72 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3_17     .      -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H5_17     .      -0.78 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7C_17    .      -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2_18     .      -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7A_18    .      -0.50 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7C_18    .      -0.48 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3_19     .      -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2_20     .      -0.40 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H5_21     .      -0.69 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6_21     .      -0.45 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7C_21    .      -0.45 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7B_22    .      -1.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7C_23    .      -0.36 eA-3
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
```

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        184 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms        184 Report
PLAT051_ALERT_1_G Mu(calc) and Mu(cif) Ratio Differs from 1.0 by .       0.65 %
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records          1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          3 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          1 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
              Au1     Au1H    Au3     Au4     Au5     S1_1    S4      S1_21
              S1_22   S1_23   C1_1    C2_1    C3_1    C4_1    C5_1    C6_1
              C7_1    C1_21   C2_21   C3_21   C4_21   C5_21   C6_21   C7_21
              C1_22   C2_22   C3_22   C4_22   C5_22   C6_22   C7_22   C1_23
              C2_23   C3_23   C4_23   C5_23   C6_23   C7_23   H2_1    H3_1
              H5_1    H6_1    H7A_1   H7B_1   H7C_1   H2_21   H3_21   H5_21
              H6_21   H7A_21  H7B_21  H7C_21  H2_22   H3_22   H5_22   H6_22
              H7A_22  H7B_22  H7C_22  H2_23   H3_23   H5_23   H6_23   H7A_23
              H7B_23  H7C_23
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)          9% Note
PLAT308_ALERT_2_G Single Bonded Metal Atom  in Structure (Unusual)        Au1 Check
PLAT308_ALERT_2_G Single Bonded Metal Atom  in Structure (Unusual)       Au1H Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H5_20    ..H2_23    .       1.17 Ang.
                                                    x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H7B_6    ..H7B_23   .       2.11 Ang.
                                               1-x,2-y,1-z  =      5_676 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in  Crystal Structure          ! Info
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.13 Ratio
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         30 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Au23      (III)     .       2.52 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Au46      (III)     .       2.58 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Au47      (III)     .       2.52 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Au49      (III)     .       2.29 Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          2 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       6078 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.454 Note
              Predicted wR2: Based on SigI**2  7.41 or SHELX Weight 28.65 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

---

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

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

PLATON version of 23/04/2026; check.def file version of 30/03/2026

---

duplicate check

No duplication found

Datablock 260112lu_zy_1226_0m - ellipsoid plot