



## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) launayite

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: launayite

---

Bond precision:	Sb- S = 0.0094 Å		Wavelength=0.71073
Cell:	a=42.6466 (14)	b=8.0381 (2)	c=34.3957 (10)
	alpha=90	beta=64.684 (2)	gamma=90
Temperature:	300 K		
	Calculated	Reported	
Volume	10658.4 (6)	10658.4 (6)	
Space group	P 2/a	P 2/a	
Hall group	-P 2ya	-P 2ya	
Moiety formula	As <sub>10.75</sub> Cu <sub>8</sub> Pb <sub>81.32</sub> S <sub>240</sub> Sb <sub>92.10</sub>	?	
Sum formula	As <sub>10.75</sub> Cu <sub>8</sub> Pb <sub>81.32</sub> S <sub>240</sub> Sb <sub>92.10</sub>	Ag <sub>0.27</sub> As <sub>12.20</sub> Cu <sub>8.37</sub> Pb <sub>81.68</sub> S <sub>240</sub> Sb <sub>90.52</sub>	
Mr	37071.13	37113.47	
Dx, g cm <sup>-3</sup>	5.776	5.782	
Z	1	1	
Mu (mm <sup>-1</sup> )	40.104	40.290	
F000	15791.8	15812.0	
F000'	15524.02		
h, k, lmax	64, 12, 51	63, 11, 51	
Nref	38470	34264	
Tmin, Tmax		0.005, 0.008	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.005 Tmax=0.008  
AbsCorr = MULTI-SCAN

Data completeness= 0.891                      Theta (max)= 32.467

R(reflections)= 0.0946( 11473)                      wR2(reflections)=  
0.3596( 34264)

S = 0.972                      Npar= 1061

---

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**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.26Ang From M'24                      4.67 eA-3

**Author Response: These kind of peaks are expected from a data set of a  
Pb-containing sulfosalt mineral with extremely weak superstructure reflections  
and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.78Ang From Pb1                      4.54 eA-3

**Author Response: These kind of peaks are expected from a data set of a  
Pb-containing sulfosalt mineral with extremely weak superstructure reflections  
and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.56Ang From Sb24                      4.46 eA-3

**Author Response: These kind of peaks are expected from a data set of a  
Pb-containing sulfosalt mineral with extremely weak superstructure reflections  
and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.79Ang From Pb4                      4.38 eA-3

**Author Response: These kind of peaks are expected from a data set of a  
Pb-containing sulfosalt mineral with extremely weak superstructure reflections  
and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.42Ang From Me20                      4.36 eA-3

**Author Response: These kind of peaks are expected from a data set of a  
Pb-containing sulfosalt mineral with extremely weak superstructure reflections  
and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.77Ang From Sb20 4.15 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.91Ang From Pb6 4.06 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.91Ang From Pb6 4.06 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.78Ang From Pb2 4.01 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.73Ang From Pb1 4.01 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.61Ang From Sb25 3.96 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 1.13Ang From Me23 3.94 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.60Ang From Pb27 3.90 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.92Ang From Pb14 3.86 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.34Ang From Sb25 3.78 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.74Ang From Pb4 3.76 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 1.04Ang From Pb12 3.75 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 1.01Ang From Pb7 3.71 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 1.80Ang From S32 3.64 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 1.08Ang From Pb4 3.63 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.97Ang From Pb10 3.63 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.95Ang From Pb26 3.62 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 1.88Ang From S55 3.61 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.88Ang From Pb7 3.61 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.59Ang From Pb12 -5.58 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.71Ang From Pb10 -5.49 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.57Ang From Pb12 -5.48 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.47Ang From Me20 -5.43 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.65Ang From As16 -5.39 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.66Ang From Sb22 -5.13 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.66Ang From Pb4 -5.07 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.74Ang From Pb10 -5.06 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.65Ang From Pb8 -5.03 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.72Ang From Pb4 -5.01 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.45Ang From As16 -4.99 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.70Ang From Pb2 -4.94 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.63Ang From Pb6 -4.90 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.72Ang From Pb7 -4.87 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.62Ang From Pb3 -4.85 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.62Ang From Pb1 -4.78 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 1.76Ang From S56 -4.77 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.60Ang From Pb3 -4.73 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.58Ang From Pb6 -4.70 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.74Ang From Pb7 -4.66 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.82Ang From Pb20 -4.65 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.64Ang From Pb5 -4.63 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.67Ang From Pb1 -4.59 eA-3

**Author Response: These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.**



PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.50Ang From As21 -4.56 eA-3

**Author Response:** These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.

PLAT972\_ALERT\_2\_A Check Calcd Resid. Dens. 0.67Ang From Pb2 -4.54 eA-3

**Author Response:** These kind of peaks are expected from a data set of a Pb-containing sulfosalt mineral with extremely weak superstructure reflections and data up to 60deg 2theta.

PLAT973\_ALERT\_2\_A Check Calcd Positive Resid. Density on Me25 4.12 eA-3



**Alert level B**

PLAT017\_ALERT\_1\_B Check Scattering Type Consistency of ME7 as SB Error?

**Author Response:** In mineralogy it is common to designate metal peaks as MeXX.

PLAT017\_ALERT\_1\_B Check Scattering Type Consistency of ME8 as PB Error?

**Author Response:** In mineralogy it is common to designate metal peaks as MeXX.

PLAT017\_ALERT\_1\_B Check Scattering Type Consistency of ME12 as PB Error?

**Author Response:** In mineralogy it is common to designate metal peaks as MeXX.

PLAT017\_ALERT\_1\_B Check Scattering Type Consistency of ME20 as SB Error?

**Author Response:** In mineralogy it is common to designate metal peaks as MeXX.

PLAT017\_ALERT\_1\_B Check Scattering Type Consistency of ME21 as SB Error?

**Author Response:** In mineralogy it is common to designate metal peaks as MeXX.

PLAT017\_ALERT\_1\_B Check Scattering Type Consistency of ME22 as SB Error?

**Author Response:** In mineralogy it is common to designate metal peaks as MeXX.

PLAT017\_ALERT\_1\_B Check Scattering Type Consistency of ME23 as SB Error?

**Author Response:** In mineralogy it is common to designate metal peaks as MeXX.

PLAT017\_ALERT\_1\_B Check Scattering Type Consistency of ME24 as SB Error?

**Author Response: In mineralogy it is common to designate metal peaks as MeXX.**

PLAT017\_ALERT\_1\_B Check Scattering Type Consistency of M'24 as SB Error?

**Author Response: In mineralogy it is common to designate metal peaks as MeXX.**

PLAT017\_ALERT\_1\_B Check Scattering Type Consistency of ME25 as SB Error?

**Author Response: In mineralogy it is common to designate metal peaks as MeXX.**

PLAT084\_ALERT\_3\_B High wR2 Value (i.e. > 0.25) ..... 0.36 Report

**Author Response: This is a superstructure with extremely weak superstructure reflections. Therefore, R-values over all reflections are high.**



#### Alert level C

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12  
Rint given 0.144

PLAT020\_ALERT\_3\_C The Value of Rint is Greater Than 0.12 ..... 0.144 Report

PLAT029\_ALERT\_3\_C \_diffn\_measured\_fraction\_theta\_full value Low . 0.966 Why?

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc: As10.75 Cu8 Pb81.32 S240 Sb92.10  
Rep.: Ag0.27 As12.20 Cu8.37 Pb81.68 S240 Sb90.52

PLAT043\_ALERT\_1\_C Calculated and Reported Mol. Weight Differ by .. 42.34 Check

PLAT053\_ALERT\_1\_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054\_ALERT\_1\_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055\_ALERT\_1\_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT068\_ALERT\_1\_C Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT077\_ALERT\_4\_C Unit-Cell Contains Non-integer Number of Atoms . Please Check

PLAT157\_ALERT\_4\_C Non-standard Monoclinic Beta Angle less 90 Deg 64.68 Degree

PLAT213\_ALERT\_2\_C Atom Me22 has ADP max/min Ratio ..... 3.2 prolat

PLAT213\_ALERT\_2\_C Atom Sb23 has ADP max/min Ratio ..... 3.4 prolat

PLAT213\_ALERT\_2\_C Atom Sb25 has ADP max/min Ratio ..... 3.2 prolat

PLAT213\_ALERT\_2\_C Atom Me23 has ADP max/min Ratio ..... 3.4 prolat

PLAT213\_ALERT\_2\_C Atom Me25 has ADP max/min Ratio ..... 3.2 prolat

PLAT213\_ALERT\_2\_C Atom Sb22 has ADP max/min Ratio ..... 3.2 prolat

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 S Ueq(max)/Ueq(min) Range 3.1 Ratio

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 Sb Ueq(max)/Ueq(min) Range 3.4 Ratio

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of Sb19 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of S58 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of S60 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of S21 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of S24 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of S35 Check

PLAT723\_ALERT\_1\_C Torsion Calc -6.00, Rep -4(22) Dev... 2.00 Sigma

S25 -PB15-AS15-S35 1\_565 1\_555 1\_555 2\_566 # 3 Check

PLAT723\_ALERT\_1\_C Torsion Calc 133.00, Rep 135(19) Dev... 2.00 Sigma

SB17-PB15-AS15-S35 1\_555 1\_555 1\_555 2\_566 # 5 Check  
 PLAT723\_ALERT\_1\_C Torsion Calc 31.00, Rep 29(26) Dev... 2.00 Sigma  
 S26 -CU2 -CU2'-S54 1\_555 1\_555 1\_555 3\_667 # 187 Check  
 PLAT723\_ALERT\_1\_C Torsion Calc -29.00, Rep -31(28) Dev... 2.00 Sigma  
 PB8 -CU2 -CU2'-S54 1\_555 1\_555 1\_555 3\_667 # 188 Check  
 PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 5.795 Check  
 PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.479 Check  
 PLAT910\_ALERT\_3\_C Missing FCF Reflection(s) Below Theta(Min)[Deg]= 2.00 Note  
 2 0 0, -2 0 1, 0 0 1, 2 0 1, 4 0 1, 0 0 2,  
 2 0 2, 4 0 2, 0 0 3, 2 0 3,  
 PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 342 Report  
 0 5 0, 0 9 0, 2 4 0, 9 9 0, 12 9 0, 15 5 0,  
 15 9 0, 16 9 0, 26 0 0, 28 0 0, -26 0 1, -24 1 1,  
 -21 4 1, -15 9 1, -14 9 1, -11 9 1, -7 9 1, -5 9 1,  
 -2 9 1, -1 9 1, 0 5 1, 0 8 1, 0 9 1, 2 4 1,  
 2 9 1, 3 9 1, 6 9 1, 10 9 1, 13 9 1, 16 9 1,  
 ( 312 More Missing: see the .ckf listing file)  
 PLAT918\_ALERT\_3\_C Reflection(s) with I(obs) much Smaller I(calc) . 7 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: Ag0.27 As12.2 Cu8.37 Pb81.68 S24  
 Atom count from the \_atom\_site data: As10.748 Cu8 Pb81.32 S240 Sb92.0  
 CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
 CELLZ01\_ALERT\_1\_G ALERT: Large difference may be due to a  
 symmetry error - see SYMMG tests  
 From the CIF: \_cell\_formula\_units\_Z 1  
 From the CIF: \_chemical\_formula\_sum Ag0.27 As12.20 Cu8.37 Pb81.68 S240  
 TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
Ag	0.27	0.00	0.27
As	12.20	10.75	1.45
Cu	8.37	8.00	0.37
Pb	81.68	81.32	0.36
S	240.00	240.00	0.00
Sb	90.52	92.10	-1.58

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 3 Note  
 PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 3 Info  
 PLAT128\_ALERT\_4\_G Alternate Setting for Input Space-group P2/a P2/n Note  
 PLAT168\_ALERT\_4\_G The CIF-Embedded .res File Contains EXYZ Records 6 Report  
 PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 25 Report  
 PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 1 Report  
 PLAT301\_ALERT\_3\_G Main Residue Disorder ..... (Resd 1) 22% Note  
 PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 10 Note  
 Me7 Me8 Me12 Me20 Me21 Me22 Me23 Me24  
 M'24 Me25  
 PLAT794\_ALERT\_5\_G Tentative Bond Valency for Pb1 (II) . 2.04 Info  
 PLAT794\_ALERT\_5\_G Tentative Bond Valency for Pb2 (II) . 1.98 Info  
 PLAT794\_ALERT\_5\_G Tentative Bond Valency for Pb3 (II) . 1.93 Info  
 PLAT794\_ALERT\_5\_G Tentative Bond Valency for Pb4 (II) . 1.84 Info  
 PLAT794\_ALERT\_5\_G Tentative Bond Valency for Pb5 (II) . 1.92 Info  
 PLAT794\_ALERT\_5\_G Tentative Bond Valency for Pb7 (II) . 1.86 Info  
 PLAT794\_ALERT\_5\_G Tentative Bond Valency for Pb9 (II) . 1.97 Info  
 PLAT794\_ALERT\_5\_G Tentative Bond Valency for Pb10 (II) . 1.91 Info

```

PLAT794_ALERT_5_G Tentative Bond Valency for Pb11      (II)      .      1.90 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb12      (II)      .      1.91 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb14      (II)      .      1.85 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb1       (III)     .      3.11 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb2       (III)     .      3.09 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb3       (III)     .      2.80 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb4       (III)     .      3.00 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb5       (III)     .      3.20 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb6       (III)     .      2.68 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb10      (III)     .      2.71 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb11      (III)     .      2.82 Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON      6 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....      4 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..      Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      3727 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File      9 Note
      2 4 1, 12 4 8, 0 8 1, 2 4 0, 3 2 4, 21 8 18,
     -2 4 11, 0 4 3, 0 4 5,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....      3.9 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      4.223 Note
      Predicted wR2: Based on SigI**2 8.52 or SHELX Weight 36.99

```

---

```

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

23 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
12 ALERT type 3 Indicator that the structure quality may be low
 8 ALERT type 4 Improvement, methodology, query or suggestion
22 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 17/09/2025; check.def file version of 17/09/2025**

---

## duplicate check

**No duplication found**

---

