

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rouxelite\_free\_o

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: rouxelite\_free\_o

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Bond precision:	Cu- S = 0.0106 Å	Wavelength=0.71073
Cell:	a=43.1883 (12)      b=8.1037 (2)      c=38.147 (1)	
	alpha=96.001 (2)      beta=116.615 (2)      gamma=95.372 (2)	
Temperature:	295 K	
	Calculated	Reported
Volume	11721.7 (6)	11721.7 (6)
Space group	C -1	C -1
Hall group	-C 1	-C 1
	Ag2.09 As1.45 Cu8 Hg3.06	
Moiety formula	01.52 Pb83.56 S261.36	?
	Sb111.84 Tl2	
	Ag2.09 As1.45 Cu8 Hg3.06	Ag0.50 As0.53 Cu2 Hg0.75 O0
Sum formula	01.52 Pb83.56 S261.36	Pb21.23 S65.43 Sb27.49
	Sb111.84 Tl2	Tl0.50
Mr	41199.12	10317.25
Dx, g cm-3	5.837	5.846
Z	1	4
Mu (mm-1)	39.593	40.004
F000	17534.3	17558.0
F000'	17236.49	
h, k, lmax	64, 12, 57	64, 12, 57
Nref	41276	55765
Tmin, Tmax		0.057, 0.069
Tmin'		

Correction method= # Reported T Limits: Tmin=0.057 Tmax=0.069  
AbsCorr = MULTI-SCAN

Data completeness= 1.351      Theta (max)= 32.173

R(reflections)= 0.0854( 17982)

wR2(reflections)=  
0.2756( 55765)

S = 0.951

Npar= 1129

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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 B

PLAT213\_ALERT\_2\_B Atom S51 has ADP max/min Ratio ..... 4.2 oblate

**Author Response: This is a disordered S atom which we couldn't properly refine as split position.**

PLAT213\_ALERT\_2\_B Atom S53 has ADP max/min Ratio ..... 4.2 oblate

**Author Response: This is a disordered S atom which we couldn't properly refine as split position.**

PLAT213\_ALERT\_2\_B Atom S65 has ADP max/min Ratio ..... 4.2 prolat

**Author Response: This is a disordered S atom which we couldn't properly refine as split position.**

PLAT213\_ALERT\_2\_B Atom S66 has ADP max/min Ratio ..... 4.2 prolat

**Author Response: This is a disordered S atom which we couldn't properly refine as split position.**

PLAT213\_ALERT\_2\_B Atom S51' has ADP max/min Ratio ..... 4.2 oblate

**Author Response: This is a disordered S atom which we couldn't properly refine as split position.**

PLAT213\_ALERT\_2\_B Atom S53' has ADP max/min Ratio ..... 4.2 oblate

**Author Response: This is a disordered S atom which we couldn't properly refine as split position.**

PLAT910\_ALERT\_3\_B Missing # of FCF Reflection(s) Below Theta(Min). 11 Note  
2 0 0, -4 0 1, -2 0 1, 0 0 1, 2 0 1, -4 0 2,  
-2 0 2, 0 0 2, 2 0 2, -2 0 3, 0 0 3,

**Author Response: This is a twinned crystal with a huge cell. Integration was difficult with many reflection overlaps. Overall the data set is 99% complete and the data to parameter ratio is excellent.**



### Alert level C

DIFMN02\_ALERT\_2\_C The minimum difference density is  $< -0.1 \times Z_{MAX} \times 0.75$   
 \_refine\_diff\_density\_min given = -6.377  
 Test value = -6.150

DIFMN03\_ALERT\_1\_C The minimum difference density is  $< -0.1 \times Z_{MAX} \times 0.75$   
 The relevant atom site should be identified.

DIFMX02\_ALERT\_1\_C The maximum difference density is  $> 0.1 \times Z_{MAX} \times 0.75$   
 The relevant atom site should be identified.

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
 Calc: Ag2.09 As1.45 Cu8 Hg3.06 O1.52 Pb83.56 S261.36  
 Sb111.84 Tl2  
 Rep.: Ag0.50 As0.53 Cu2 Hg0.75 O0 Pb21.23 S65.43 Sb2  
 7.49 Tl0.50

PLAT043\_ALERT\_1\_C Calculated and Reported Mol. Weight Differ by .. 69.88 Check

PLAT051\_ALERT\_1\_C Mu(calc) and Mu(cif) Ratio Differs from 1.0 by . 1.03 %

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

PLAT084\_ALERT\_3\_C High wR2 Value (i.e.  $> 0.25$ ) ..... 0.28 Report

PLAT097\_ALERT\_2\_C Large Reported Max. (Positive) Residual Density 6.73 eA-3

PLAT098\_ALERT\_2\_C Large Reported Min. (Negative) Residual Density -6.38 eA-3

PLAT155\_ALERT\_4\_C The Triclinic Unit Cell is NOT Reduced ..... Please Do !

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 S Ueq(max)/Ueq(min) Range 3.9 Ratio

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of S64 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Sb16 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Sb19 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 S42 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of S55 Check

PLAT723\_ALERT\_1\_C Torsion Calc 20.00, Rep 23(22) Dev... 3.00 Sigma

SB23-PB28-ME28-S7 1\_555 1\_555 1\_555 4\_556 # 344 Check

PLAT723\_ALERT\_1\_C Torsion Calc 136.00, Rep 139(21) Dev... 3.00 Sigma

SB23-PB28-ME28-S37 1\_555 1\_555 1\_555 1\_545 # 437 Check

PLAT723\_ALERT\_1\_C Torsion Calc -20.00, Rep -23(22) Dev... 3.00 Sigma

S7 -PB28-ME28-SB23 4\_556 1\_555 1\_555 1\_555 # 443 Check

PLAT723\_ALERT\_1\_C Torsion Calc -136.00, Rep -139(21) Dev... 3.00 Sigma

S37 -PB28-ME28-SB23 1\_545 1\_555 1\_555 1\_555 # 448 Check

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 9.701 Check

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 3.540 Check

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 235 Report

31 -1 0, 38 -6 0, 40 -6 0, -40 6 1, -32 2 1, -31 1 1,  
 20 0 1, 31 -1 1, 38 -6 1, -40 6 2, -32 0 2, -32 2 2,  
 -31 -1 2, -31 1 2, -30 0 2, -28 0 2, 14 4 2, 20 4 2,  
 30 -2 2, 30 0 2, -40 6 3, -32 0 3, -32 2 3, -31 -1 3,  
 -30 0 3, -28 0 3, -26 0 3, -24 0 3, 12 -4 3, 22 -4 3,  
 30 -2 3, -40 6 4, -33 1 4, -32 0 4, -32 2 4, -31 -1 4,  
 -30 0 4, -28 0 4, -26 0 4, 16 0 4, 22 0 4, 24 6 4,

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-42  6  5, -34  2  5, -33  1  5, -32  0  5, -31 -1  5, -30 -2  5,
-30  0  5, -28  0  5,  20  2  5,  24  6  5,  26  6  5,  28 -2  5,
 28  0  5, -42  6  6, -33  1  6, -32  0  6, -31 -1  6, -30 -2  6,
-30  0  6, -16  0  6, -12  6  6,  4  2  6,  24  6  6,  26  6  6,
 28 -2  6,  30  2  6, -42  6  7, -40  6  7, -33  1  7, -32  0  7,
-31 -1  7, -30 -2  7, -30  0  7, -16  6  7, -14  6  7, -12  6  7,
 22 -2  7,  22  6  7,  24  6  7,  26 -2  7,  26  6  7, -34  0  8,
-33 -1  8, -33  1  8, -32  0  8, -31 -1  8, -30 -2  8,  6 -2  8,
 22  6  8,  26 -2  8,  32 -2  8, -34  0  9, -33 -1  9, -32 -2  9,
PLAT992_ALERT_5_C Repd & Actual _reflns_number_gt Values Differ by      13 Check

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## 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: Ag0.5 As0.53 Cu2 Hg0.75 Pb21.23  
     Atom count from the \_atom\_site data: Ag0.522 As0.363 Cu2 Hg0.766 O0.3  
 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      4  
     From the CIF: \_chemical\_formula\_sum Ag0.50 As0.53 Cu2 Hg0.75 O0 Pb21.2  
     TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
Ag	2.00	2.09	-0.09
As	2.12	1.45	0.67
Cu	8.00	8.00	0.00
Hg	3.00	3.06	-0.06
O	4.00	1.52	2.48
Pb	84.92	83.56	1.36
S	261.72	261.36	0.36
Sb	109.96	111.84	-1.88
Tl	2.00	2.00	0.00

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      10 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension      3 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of ME17 as PB
PLAT017_ALERT_1_G Check Scattering Type Consistency of ME18 as PB
PLAT017_ALERT_1_G Check Scattering Type Consistency of ME19 as SB
PLAT017_ALERT_1_G Check Scattering Type Consistency of ME22 as SB
PLAT017_ALERT_1_G Check Scattering Type Consistency of ME27 as SB
PLAT017_ALERT_1_G Check Scattering Type Consistency of ME28 as SB
PLAT017_ALERT_1_G Check Scattering Type Consistency of ME20 as SB
PLAT017_ALERT_1_G Check Scattering Type Consistency of ME21 as SB
PLAT017_ALERT_1_G Check Scattering Type Consistency of ME23 as SB
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.250 Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C-1 P-1 Note
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 5 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 18 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at ..... 0.5 Check
Pb12 Tl12
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 14% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 9 Note
Me17 Me18 Me19 Me22 Me27 Me28 Me20 Me21
Me23

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PLAT794_ALERT_5_G	Tentative Bond Valency for Pb5	(II)	.	1.98	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb7	(II)	.	2.00	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb8	(II)	.	1.96	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb9	(II)	.	1.81	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb10	(II)	.	1.82	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb11	(II)	.	1.96	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb13	(II)	.	1.88	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb14	(II)	.	2.06	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb15	(II)	.	1.82	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Pb16	(II)	.	1.79	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb1	(III)	.	3.07	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb4	(III)	.	3.39	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb5	(III)	.	3.00	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb7	(III)	.	2.91	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb8	(III)	.	2.68	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb10	(III)	.	3.18	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb11	(III)	.	3.08	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb12	(III)	.	2.90	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb13	(III)	.	2.45	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb14	(III)	.	3.08	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb15	(III)	.	2.66	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb17	(III)	.	3.19	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb18	(III)	.	2.83	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb25	(III)	.	2.45	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb26	(III)	.	2.73	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....			8	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..			!	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..			Please Do !	
PLAT908_ALERT_2_G	Max. Perc. Data with I > 2*s(I) per Res.Shell .			66.41%	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600			2957	Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law ( 1-2 1) Est.d BASF			0.53	Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law [ 0-1 0] Est.d BASF			0.47	Check
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			52	Note
	-38 -2 1, -28 4 2, -26 -2 19, -26 0 4, -24 4 22, -22 0 24,				
	-18 -4 1, -18 2 9, -18 2 10, -16 -2 11, -16 -2 12, -16 0 6,				
	-16 0 12, -16 0 27, -16 2 10, -14 -2 13, -12 2 15, -12 2 26,				
	-10 -2 1, -10 -2 17, -10 -2 28, -10 2 25, -8 -4 1, -8 -2 27,				
	-8 4 15, -8 4 16, -6 0 17, -6 0 26, -4 -4 19, -4 -4 20,				
	2 0 11, 4 2 6, 6 -2 8, 10 -2 22, 10 0 21, 12 -4 3,				
	12 -2 1, 12 0 10, 12 0 14, 14 -4 10, 14 4 2, 16 0 4,				
	18 -4 6, 20 0 1, 20 2 5, 20 4 2, 22 -4 3, 22 -2 7,				
	22 0 4, 26 0 15,				
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....			1.5	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....			2.892	Note
	Predicted wR2: Based on SigI**2 9.53 or SHELX Weight 28.98				

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 7 **ALERT level B** = A potentially serious problem, consider carefully  
 30 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 58 **ALERT level G** = General information/check it is not something unexpected
- 27 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 20 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 8 ALERT type 3 Indicator that the structure quality may be low  
 10 ALERT type 4 Improvement, methodology, query or suggestion  
 30 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. 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.

Datablock rouxelite\_free\_o - ellipsoid plot

