



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: I

Bond precision:	Tl- S = 0.0050 Å		Wavelength=0.71073
Cell:	a=15.791 (8)	b=10.000 (5)	c=6.323 (3)
	alpha=90	beta=99.25 (2)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	985.5 (8)	985.5 (8)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	As ₄ Cu ₄ S ₁₀ Tl ₂ , 2 (Tl)	?	
Sum formula	As ₄ Cu ₄ S ₁₀ Tl ₄	As ₂ Cu ₂ S ₅ Tl ₂	
Mr	1692.00	845.96	
Dx, g cm ⁻³	5.702	5.702	
Z	2	4	
Mu (mm ⁻¹)	44.509	44.510	
F000	1464.0	1464.0	
F000'	1449.92		
h, k, lmax	28, 18, 11	28, 18, 11	
Nref	6153	6057	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.984

Theta(max)= 40.106

R(reflections)= 0.1218(4753)

wR2(reflections)=
0.3604(6057)

S = 1.151

Npar= 101

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

EXPT005_ALERT_1_A _exptl_crystal_description is missing

Crystal habit description.

The following tests will not be performed.

CRYSR_01

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing

Diffractometer make and type. Replaces _diffrn_measurement_type.

PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used Value Please Do !

PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value Please Do !

PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value Please Do !

PLAT699_ALERT_1_A Missing _exptl_crystal_description Value Please Do !

Alert level B

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.36 Report

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 12.15 eA-3

PLAT213_ALERT_2_B Atom As1 has ADP max/min Ratio 4.6 prolat

Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75

_refine_diff_density_min given = -7.779

Test value = -6.075

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75

The relevant atom site should be identified.

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 0.163

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.163 Report

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

Calc: As4 Cu4 S10 Tl4

Rep.: As2 Cu2 S5 Tl2

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !

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

PLAT082_ALERT_2_C High R1 Value 0.12 Report

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -7.78 eA-3

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.6 Note

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	95.00	Why ?
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Tl1 (I) .	1.01	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Tl2 (I) .	1.00	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
	1 0 0,		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.3	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check

6 **ALERT level A** = Most likely a serious problem - resolve or explain
 3 **ALERT level B** = A potentially serious problem, consider carefully
 13 **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

17 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 9 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
 0 ALERT type 4 Improvement, methodology, query or suggestion
 3 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 26/09/2025; check.def file version of 20/09/2025

Datablock 1 - ellipsoid plot

