

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) shelx

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](#)

Please wait while processing [Interpreting this report](#)

[Structure factor report](#)

Datablock: shelx

Bond precision: Cu- S = 0.0030 Å Wavelength=0.71073
 Cell: a=10.5663(12) b=10.5663(12) c=10.5663(12)
 alpha=90 beta=90 gamma=90
 Temperature: 293 K

	Calculated	Reported
Volume	1179.7(4)	1179.7(4)
Space group	I -4 3 m	I -4 3 m
Hall group	I -4 2 3	I -4 2 3
Moiety formula	Ag8.04 Cu15.94 S26 Sb8	?
Sum formula	Ag8.04 Cu15.94 S26 Sb8	Ag4.02 Cu7.97 S13 Sb4
Mr	3687.65	1843.82
Dx, g cm-3	5.191	5.191
Z	1	2
Mu (mm-1)	15.903	15.903
F000	1664.0	1664.0
F000'	1660.81	
h,k,lmax	15,15,15	11,15,12
Nref	391[223]	384
Tmin,Tmax	0.470,0.621	0.429,0.746
Tmin'	0.434	

Correction method= # Reported T Limits: Tmin=0.429 Tmax=0.746 AbsCorr = MULTI-SCAN

Data completeness= 1.72/0.98 Theta(max)= 31.255

R(reflections)= 0.0381(370) wR2(reflections)= 0.0812(384)

S = 1.245 Npar= 22

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

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.00Ang From S2 -4.48 eA-3

🟡Alert level B

PLAT220_ALERT_2_B NonSolvent Resd 1 S Ueq(max)/Ueq(min) Range 9.1 Ratio

PLAT924_ALERT_1_B The Reported and Calculated Rho(min) Differ by . 2.54 eA-3

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.57Ang From S2 2.64 eA-3

🟢Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.044 Check

PLAT925_ALERT_1_C The Reported and Calculated Rho(max) Differ by . 1.01 eA-3

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.73Ang From Sb 1.60 eA-3

●Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT017_ALERT_1_G	Check Scattering Type Consistency of M2A as	AG	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of M2B as	CU	
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.5000	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	28.17	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	28%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	3	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb (III) .	3.32	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	2	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	4	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	3	Units
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by .	3	Units
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check

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

- 9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 7 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
 3 ALERT type 4 Improvement, methodology, query or suggestion
 4 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. 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

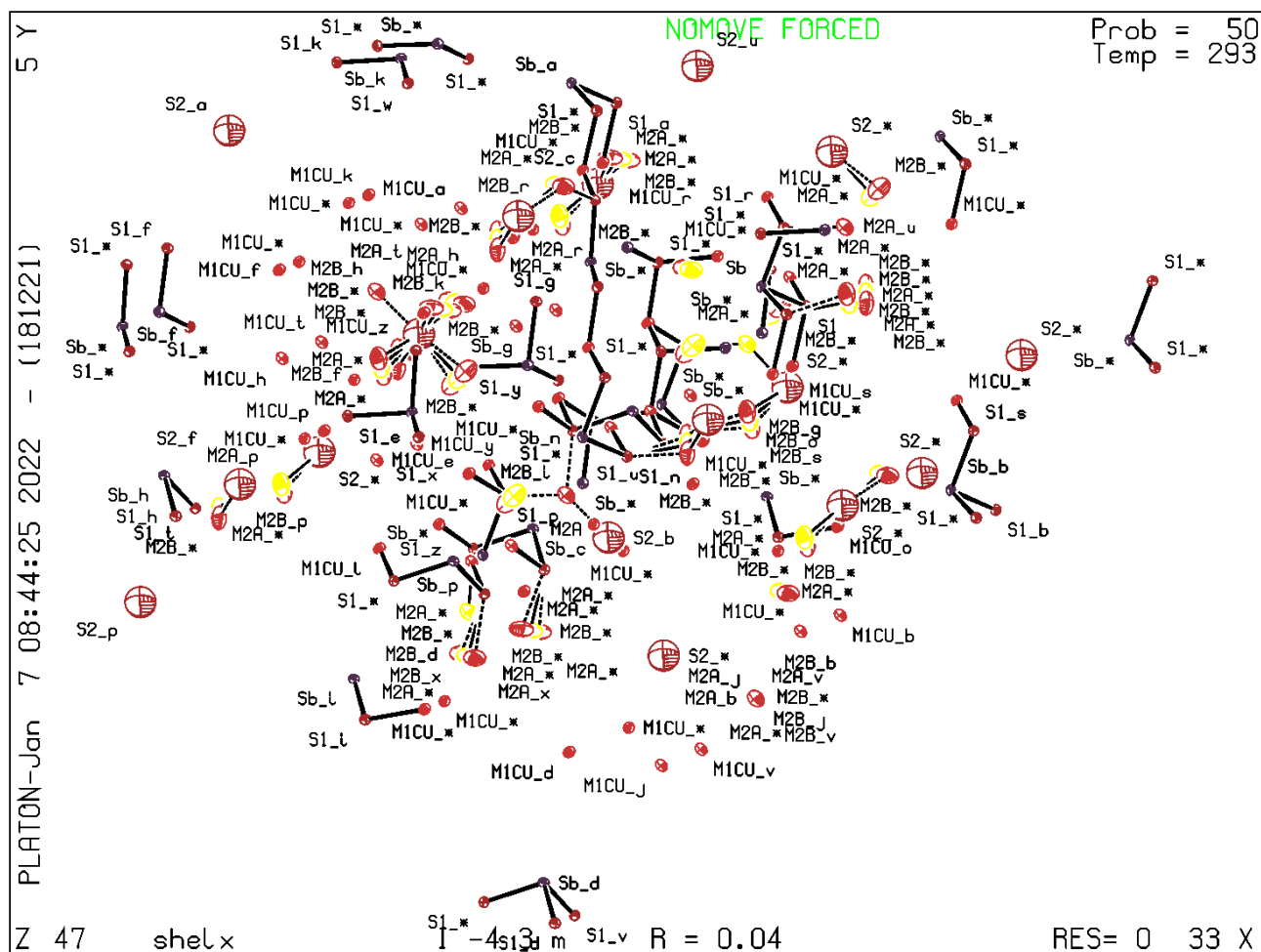
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 18/12/2021; check.def file version of 18/12/2021

Datablock shelx - ellipsoid plot



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