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:	= 0.0000 A		Wavelength=0.71073
Cell:	a=10.1710(8)	b=10.1710(8)	c=10.1710(8)
	alpha=90	beta=90	gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	1052.2(2)	1052.2(2)
Space group	I -4 3 m	I -4 3 m
Hall group	I -4 2 3	I -4 2 3
Moiety formula	As7.58 Cu22.33 Fe1.68 S26 Sb0.42	?
Sum formula	As7.58 Cu22.33 Fe1.68 S26 Sb0.42	As3.775 Cu11.90 S13 Sb0.225
Mr	2965.81	1483.07
Dx,g cm-3	4.681	4.681
Z	1	2
Mu (mm-1)	19.051	19.211
F000	1378.9	1378.1
F000'	1390.43	
h,k,lmax	13,13,13	12,13,11
Nref	280[162]	279
Tmin,Tmax	0.414,0.562	0.613,0.746
Tmin'	0.304	

Correction method= # Reported T Limits: Tmin=0.613 Tmax=0.746 AbsCorr =
MULTI-SCAN

Data completeness= 1.72/1.00   Theta(max)= 28.790

R(reflections)= 0.0178(263)   wR2(reflections)= 0.0375(279)

S = 0.968   Npar= 24

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 C

PLAT031_ALERT_4_C Refined Extinction Parameter Within Range of ...   2.786 Sigma
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..   Please Check
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ....   6.71 Note

⚪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:As3.775 Cu11.9 S13 Sb0.225
        Atom count from the _atom_site data: As3.788 Cu11.166 Fe0.84 S13 Sb0.
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   2
From the CIF: _chemical_formula_sum As3.775 Cu11.90 S13 Sb0.225
TEST: Compare cell contents of formula and atom_site data
WARNING: Unexpected atom type is in site list: Fe
WARNING: Formula and atom_type_symbol element names mismatch.

atom	Z*formula	cif sites	diff
As	7.55	7.58	-0.03
Cu	23.80	22.33	1.47
S	26.00	26.00	0.00
Sb	0.45	0.42	0.03

WARNING: Site labels do not match formula elements

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   3 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2A   as   CU
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2B   as   CU
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0   0.995 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.5000 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records   2 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   3 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =   3 Note
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)   75% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   6 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....   ! 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
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....   1 Note
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.   2 Units
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .   2 Units
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged   Please Check

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

12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 2 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
 6 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. 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.

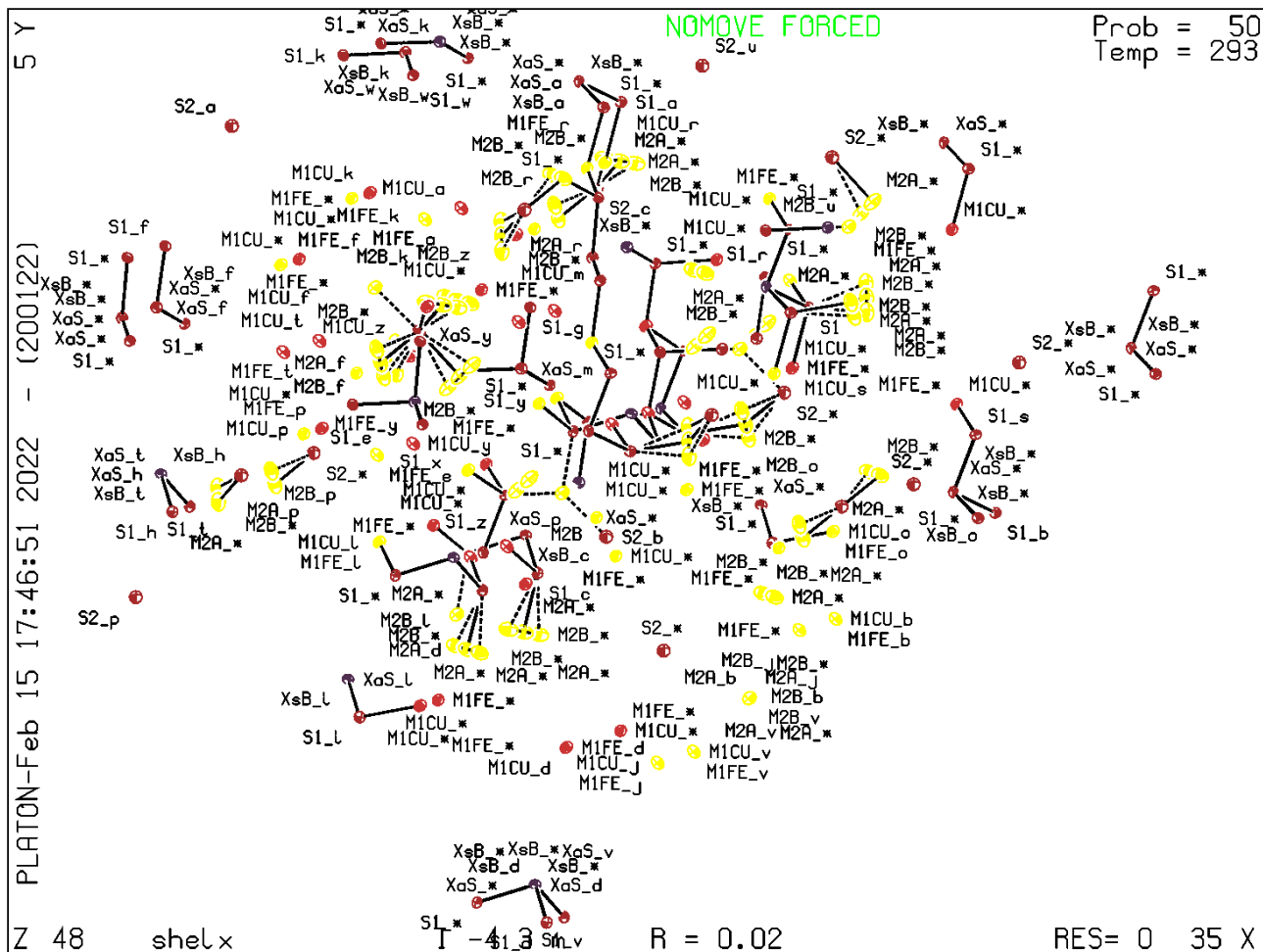**Publication of your CIF in IUCr journals**

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 20/01/2022; check.def file version of 19/01/2022

Datablock shelx - ellipsoid plot