

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=10.5505(10) b=10.5505(10) c=10.5505(10)	
	alpha=90 beta=90 gamma=90	
Temperature:	293 K	

	Calculated	Reported
Volume	1174.4(3)	1174.4(3)
Space group	I -4 3 m	I -4 3 m
Hall group	I -4 2 3	I -4 2 3
Moiety formula	Ag6.24 As0.40 Cu17.76 S26 Sb7.60	?
Sum formula	Ag6.24 As0.40 Cu17.76 S26 Sb7.60	Ag3.12 As0.20 Cu8.88 S13 Sb3.80
Mr	3590.66	1795.33
Dx, g cm-3	5.077	5.077
Z	1	2
Mu (mm-1)	16.104	16.104
F000	1625.1	1625.1
F000'	1624.35	
h,k,lmax	15,15,15	13,13,13
Nref	423[241]	358
Tmin,Tmax	0.466,0.569	0.464,0.746
Tmin'	0.443	

Correction method= # Reported T Limits: Tmin=0.464 Tmax=0.746 AbsCorr = MULTI-SCAN

Data completeness= 1.49/0.85 Theta(max)= 32.179

R(reflections)= 0.0351(327) wR2(reflections)= 0.0537(358)

S = 1.163 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 B

[PLAT220_ALERT_2_B](#) NonSolvent Resd 1 S Ueq(max)/Ueq(min) Range 8.2 Ratio
[PLAT972_ALERT_2_B](#) Check Calcd Resid. Dens. 0.00Ang From S2 -2.94 eA-3

●Alert level C

[PLAT029_ALERT_3_C](#) diffrn_measured_fraction_theta_full value Low . 0.977 Why?
[PLAT077_ALERT_4_C](#) Unitcell Contains Non-integer Number of Atoms .. Please Check
[PLAT924_ALERT_1_C](#) The Reported and Calculated Rho(min) Differ by . 1.24 eA-3
[PLAT971_ALERT_2_C](#) Check Calcd Resid. Dens. 0.55Ang From S2 1.72 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

And 2 other PLAT017 Alerts

More ...

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	10.69	Why ?
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	1	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	50%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	3	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).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	10	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	2	Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ	2	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ	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 explain2 **ALERT level B** = A potentially serious problem, consider carefully4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight23 **ALERT level G** = General information/check it is not something unexpected

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

6 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

5 ALERT type 4 Improvement, methodology, query or suggestion

5 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

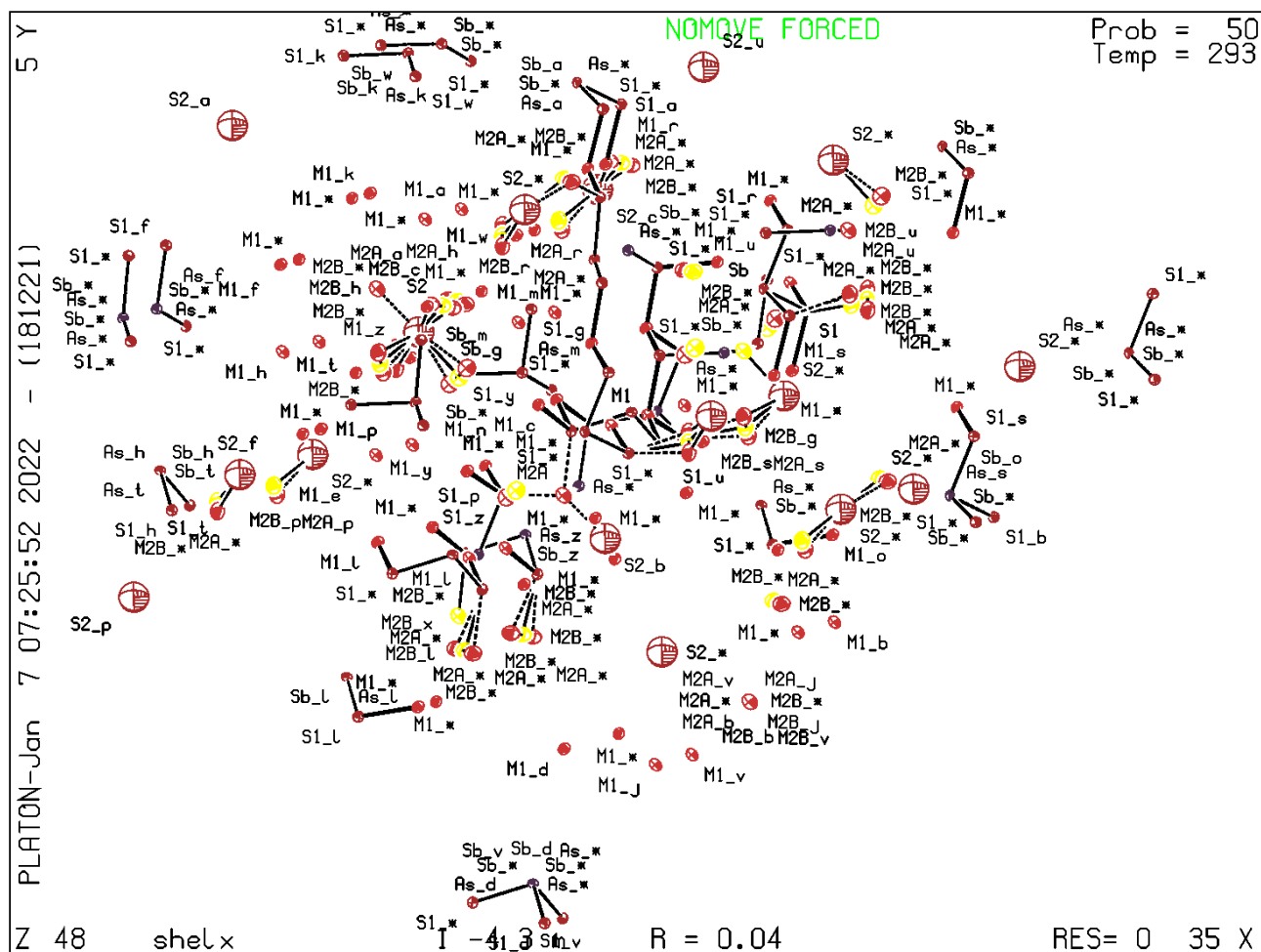
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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