

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 Å	Wavelength=0.71073
Cell:	a=10.5155(13) b=10.5155(13) c=10.5155(13)	
	alpha=90 beta=90 gamma=90	
Temperature:	293 K	

	Calculated	Reported
Volume	1162.8(4)	1162.8(4)
Space group	I -4 3 m	I -4 3 m
Hall group	I -4 2 3	I -4 2 3
Moiety formula	Ag6.48 As1.92 Cd0.48 Cu17 S26 Sb6.08	?
Sum formula	Ag6.48 As1.92 Cd0.48 Cu17 S26 Sb6.08	Ag3.24 As0.96 Cd0.24 Cu8.50 S13 Sb3.04
Mr	3550.50	1775.25
Dx, g cm-3	5.070	5.070
Z	1	2
Mu (mm-1)	16.444	16.444
F000	1609.8	1609.8
F000'	1609.17	
h,k,lmax	15,15,15	15,12,14
Nref	391[223]	388
Tmin,Tmax	0.108,0.228	0.438,0.746
Tmin'	0.032	

Correction method= # Reported T Limits: Tmin=0.438 Tmax=0.746 AbsCorr = MULTI-SCAN

Data completeness= 1.74/0.99 Theta(max)= 31.423

R(reflections)= 0.0297(385) wR2(reflections)= 0.0692(388)

S = 1.282 Npar= 23

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 7.4 Ratio
 PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.00Ang From S2 -2.79 eA-3

●Alert level C

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
 PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report
 PLAT924_ALERT_1_C The Reported and Calculated Rho(min) Differ by . 1.68 eA-3
 PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.57Ang From S2 2.22 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
 PLAT019_ALERT_1_G _diffn_measured_fraction_theta_full/*_max < 1.0 0.987 Report
 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 17.99 Why ?
 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
 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) 75% Note
 PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 4 Note
 PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
 PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 with s.u. 0.08 Check
 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 3 Note
 PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 3 Units
 PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units
 PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 2 **ALERT level B** = A potentially serious problem, consider carefully
 4 **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
 4 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
 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

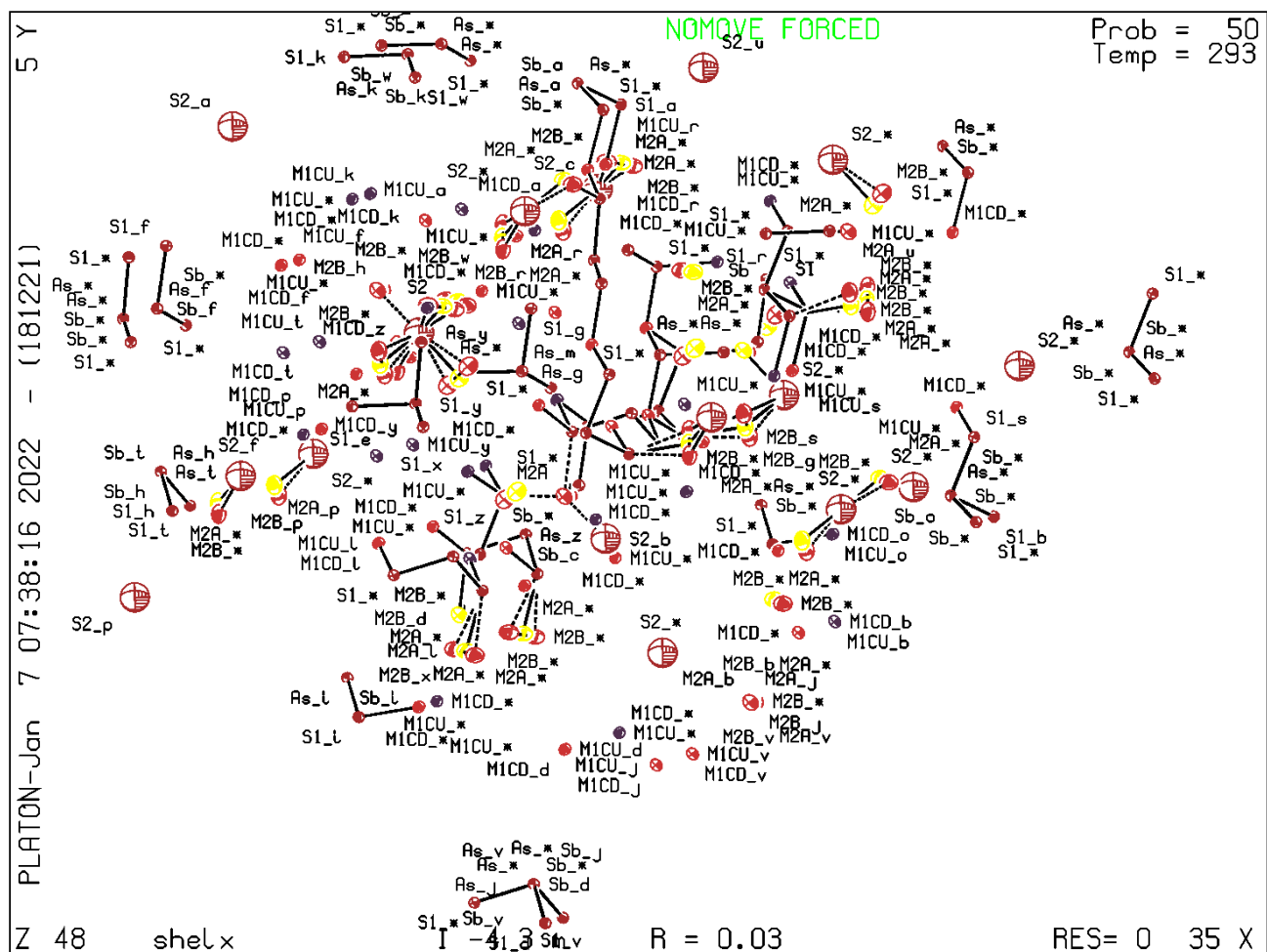
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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