

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 = 0.0016 Å	Wavelength=0.71073
Cell:	a=7.9681(2) b=9.7452(3) c=10.0710(3)	
	alpha=77.759(1) beta=76.990(1) gamma=79.422(1)	
Temperature: 293 K		

	Calculated	Reported
Volume	737.01(4)	737.01(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Cu10 Hg3 S8	?
Sum formula	Cu10 Hg3 S8	Cu10 Hg3 S8
Mr	1493.75	1493.65
Dx, g cm ⁻³	6.731	6.731
Z	2	2
Mu (mm ⁻¹)	46.310	46.311
F000	1316.0	1316.0
F000'	1312.12	
h,k,lmax	11,14,14	11,14,14
Nref	4720	4709
Tmin,Tmax	0.125,0.249	0.125,0.249
Tmin'	0.054	

Correction method= # Reported T Limits: Tmin=0.125 Tmax=0.249 AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 31.035

R(reflections)= 0.0262(4212) wR2(reflections)= 0.0702(4709)

S = 1.033 Npar= 193

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

[PLAT972_ALERT_2_B](#) Check Calcd Resid. Dens. 0.72Ang From Cu1 -2.62 eA-3

🟡Alert level C

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	Cu1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	Cu6 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	S5 Check

And 3 other PLAT242 Alerts

[More ...](#)

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	4 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.29Ang From Cu1	1.87 eA-3

And 3 other PLAT971 Alerts

More ...

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.74Ang From Cu2 -1.71 eA-3

PLAT974_ALERT_2_C Check Calcd Negative Resid. Density on Cu1 -1.26 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.63 Why ?

PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem a/2 86 %Fit

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree

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 Cu7 (I) . 1.02 Info

And 3 other PLAT794 Alerts

More ...

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 7 Note

PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain1 **ALERT level B** = A potentially serious problem, consider carefully14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight14 **ALERT level G** = General information/check it is not something unexpected

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

16 ALERT type 2 Indicator that the structure model may be wrong or deficient

2 ALERT type 3 Indicator that the structure quality may be low

1 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

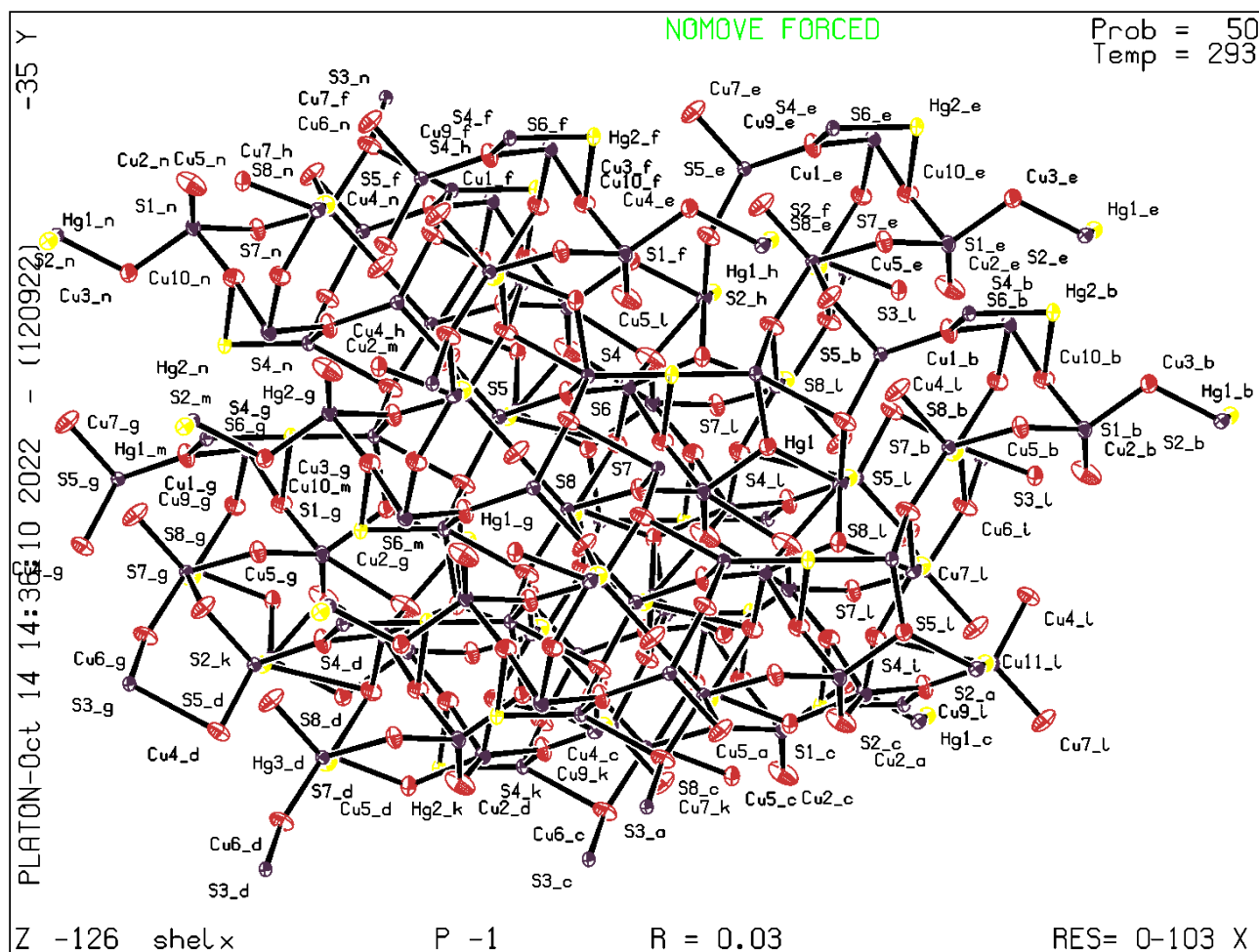
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 12/09/2022; check.def file version of 09/08/2022

Datablock shelx - ellipsoid plot



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