

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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 Interpreting this report

Datablock: 2

Bond precision: C-C = 0.0079 Å

Wavelength=0.71073

Cell: a=6.1916(6) b=8.1504(8) c=12.7804(13)
 alpha=95.079(3) beta=103.019(3) gamma=106.241(3)
Temperature: 293 K

	Calculated	Reported
Volume	595.33(10)	595.33(10)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C22 H30 Cu N6 O6	?
Sum formula	C22 H30 Cu N6 O6	C22 H34 Cu N6 O6
Mr	538.07	542.09
Dx, g cm-3	1.501	1.512
Z	1	1
Mu (mm-1)	0.968	0.969
F000	281.0	285.0
F000'	281.43	
h, k, lmax	8, 10, 16	8, 10, 16
Nref	2747	2674
Tmin, Tmax	0.840, 0.908	0.789, 0.820
Tmin'	0.824	

Correction method= # Reported T Limits: Tmin=0.789 Tmax=0.820
AbsCorr = MULTI-SCAN

Data completeness= 0.973

Theta(max)= 27.550

R(reflections)= 0.0697(2228)

wR2(reflections)= 0.1804(2674)

S = 1.110

Npar= 158

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

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full value Low .	0.973	Note
PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ		Please Check
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..	4.02	Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT161_ALERT_4_C	Missing or Zero s.u. (esd) on x-coordinate for .	01W	Check
PLAT162_ALERT_4_C	Missing or Zero s.u. (esd) on y-coordinate for .	01W	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	01W	Check
PLAT165_ALERT_3_C	Nr. of Status R Flagged Non-Hydrogen Atoms	1	Note
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00786	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact H16B .. H18 ..	1.91	Ang.

● 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: C22 H34 Cu1 N6 O6
Atom count from the _atom_site data: C22 H30 Cu1 N6 O6

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 1
From the CIF: _chemical_formula_sum C22 H34 Cu N6 O6
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	22.00	22.00	0.00
H	34.00	30.00	4.00
Cu	1.00	1.00	0.00
N	6.00	6.00	0.00
O	6.00	6.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF		Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as		mixed Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003	Degree
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	293	Check
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	3	Do !
	N1 -CU1 -N1 -C7 2.00 0.00 2.665 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	7	Do !
	N1 -CU1 -N1 -C6 14.00 0.00 2.665 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	11	Do !
	N1 -CU1 -N1 -C15 10.00 0.00 2.665 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	37	Do !
	O2 -CU1 -O2 -C3 16.00 0.00 2.665 1.555 1.555	1.555	
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	2	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note

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

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
9 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

