

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: 1

Bond precision: C-C = 0.0063 Å

Wavelength=0.71073

Cell: a=13.4647(13) b=16.7473(18) c=18.793(2)
 alpha=109.221(2) beta=96.022(2) gamma=98.901(2)
Temperature: 113 K

	Calculated	Reported
Volume	3897.8(7)	3897.9(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C118 H70 Cu7 F84 N10 O36, 3(C0.50 H1.50)	C120 H76 Cu7 F84 N10 O36
Sum formula	C120 H76 Cu7 F84 N10 O36	C120 H76 Cu7 F84 N10 O36
Mr	4274.76	4274.76
Dx,g cm-3	1.821	1.821
Z	1	1
Mu (mm-1)	1.113	1.113
F000	2113.0	2113.0
F000'	2117.21	
h,k,lmax	16,19,22	16,19,22
Nref	13715	13415
Tmin,Tmax	0.800,0.837	0.800,0.837
Tmin'	0.800	

Correction method= # Reported T Limits: Tmin=0.800 Tmax=0.837

AbsCorr = MULTI-SCAN

Data completeness= 0.978

Theta(max)= 25.000

R(reflections)= 0.0497(10282)

wR2(reflections)= 0.1512(13415)

S = 0.984

Npar= 1210

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	0.978	Why?
PLAT213_ALERT_2_C	Atom C20	has ADP max/min Ratio	3.9	prolat
PLAT215_ALERT_3_C	Disordered C27	has ADP max/min Ratio	3.3	Note
PLAT220_ALERT_2_C	NonSolvent Resd 1 C	Ueq(max)/Ueq(min) Range	5.8	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 1 F	Ueq(max)/Ueq(min) Range	4.9	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H	Uiso(max)/Uiso(min) Range	6.7	Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C55	Check	
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00631	Ang.	



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	11	Note	
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	13	Report	
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info	
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ	Please	Check	
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check	
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree	
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	12	Report	
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	9	Report	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C29	Check	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C33	Check	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C34	Check	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C38	Check	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C39	Check	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C43	Check	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C44	Check	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C48	Check	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C49	Check	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C53	Check	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C58	Check	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C59	Check	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C60	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of C22	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C27	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C25	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C26	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26B	Constrained at	0.5	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H26C	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	2%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 3)	100%	Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H27B ..H28A .	1.83	Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H27C ..H28A .	1.81	Ang.
		x,y,z =	1_555	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn	H26A ..H28B .	2.00	Ang.
		x,y,z =	1_555	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn	H26A ..H28C .	1.86	Ang.
		x,y,z =	1_555	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn	H26B ..H28B .	2.00	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	N4 ..C26	2.45	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	N5 ..C25	2.44	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	N5 ..C26	2.93	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C19 ..C26	3.00	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C19 ..C25	3.18	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C20 ..C26	1.83	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C20 ..C25	2.35	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C21 ..C25	1.80	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C21 ..C26	2.21	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C26 ..C28	2.14	Ang.
		x,y,z =	1_555	Check
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C20	--C27	1.75	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C20	--C26	1.84	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C21	--C25	1.80	Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1	(II) .	2.23	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu2	(II) .	2.15	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu3	(II) .	2.25	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		90	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .			Please Do !
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		2.7	Low
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
 8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 73 **ALERT level G** = General information/check it is not something unexpected

4 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
 38 **ALERT type 2** Indicator that the structure model may be wrong or deficient
 7 **ALERT type 3** Indicator that the structure quality may be low
 28 **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.

