

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ras1806SNQ

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: ras1806SNQ

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Bond precision:    C-C = 0.0030 Å                      Wavelength=1.54184

Cell:                      a=10.2326(2)      b=13.2639(2)                      c=13.1667(2)  
                            alpha=90                      beta=103.6655(14)                      gamma=90  
Temperature:      150 K

	Calculated	Reported
Volume	1736.45(5)	1736.45(5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C14 H19 Cl Cu N2 O6, H2 O	C14 H19 Cl Cu N2 O6, H2 O
Sum formula	C14 H21 Cl Cu N2 O7	C14 H21 Cl Cu N2 O7
Mr	428.33	428.33
Dx,g cm-3	1.638	1.638
Z	4	4
Mu (mm-1)	3.560	3.560
F000	884.0	884.0
F000'	880.10	
h,k,lmax	12,16,16	12,16,16
Nref	3527	3505
Tmin,Tmax	0.749,0.822	0.620,0.820
Tmin'	0.372	

Correction method= # Reported T Limits: Tmin=0.620 Tmax=0.820  
AbsCorr = MULTI-SCAN

Data completeness= 0.994                      Theta(max)= 73.955

R(reflections)= 0.0337( 3346)                      wR2(reflections)= 0.0870( 3505)

S = 1.007                      Npar= 272

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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.

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**Alert level A**

PLAT902\_ALERT\_1\_A No (Interpretable) Reflections Found in FCF .... Please Check

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**Alert level C**

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Cl1 Check

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**Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	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 .....	2	Report
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	9	Note
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1 --O1 .	5.7	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1 --N2 .	5.9	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of H1	Constrained at	0.849 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H41	Constrained at	0.849 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42	Constrained at	0.849 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H51	Constrained at	0.849 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52	Constrained at	0.849 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H131	Constrained at	0.849 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H132	Constrained at	0.849 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H141	Constrained at	0.849 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H142	Constrained at	0.849 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9131	Constrained at	0.151 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9132	Constrained at	0.151 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5	Constrained at	0.151 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43	Constrained at	0.151 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H44	Constrained at	0.151 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H143	Constrained at	0.151 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H144	Constrained at	0.151 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H951	Constrained at	0.151 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H952	Constrained at	0.151 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	13%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	2	Note
PLAT793_ALERT_4_G	Model has Chirality at N2 (Centro SPGR)	S	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	10	Note

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

1 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  
2 ALERT type 3 Indicator that the structure quality may be low  
21 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

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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.

