

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) RB21082f

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: RB21082f

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Bond precision:	Cu- O = 0.0009 A	Wavelength=0.71073
Cell:	a=8.0553 (3) alpha=90	b=3.7295 (2) beta=90
		c=7.3674 (3) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	221.333 (17)	221.333 (17)
Space group	P m n a	P m n a
Hall group	-P 2ac 2	-P 2ac 2
Moiety formula	C12 Cu H4 O2	C12 Cu H4 O2
Sum formula	C12 Cu H4 O2	C12 Cu H4 O2
Mr	170.48	170.48
Dx, g cm <sup>-3</sup>	2.558	2.558
Z	2	2
Mu (mm <sup>-1</sup> )	5.967	5.967
F000	166.0	167.4
F000'	167.28	
h, k, lmax	12, 5, 11	12, 5, 11
Nref	499	499
Tmin, Tmax	0.762, 0.888	0.277, 1.000
Tmin'	0.284	

Correction method= # Reported T Limits: Tmin=0.277 Tmax=1.000  
AbsCorr = GAUSSIAN

Data completeness= 1.000      Theta (max)= 34.470

R(reflections)= 0.0119 ( 476)	wR2(reflections)= 0.0245 ( 499)
S = 1.062	Npar= 25

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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 G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II)	2.08	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	6	Note
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	69.0	Degree
PLAT979_ALERT_1_G	NoSpherA2 Scattering Factors Used .....		Please Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
8 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
0 ALERT type 2 Indicator that the structure model may be wrong or deficient  
1 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
3 ALERT type 5 Informative message, check
-

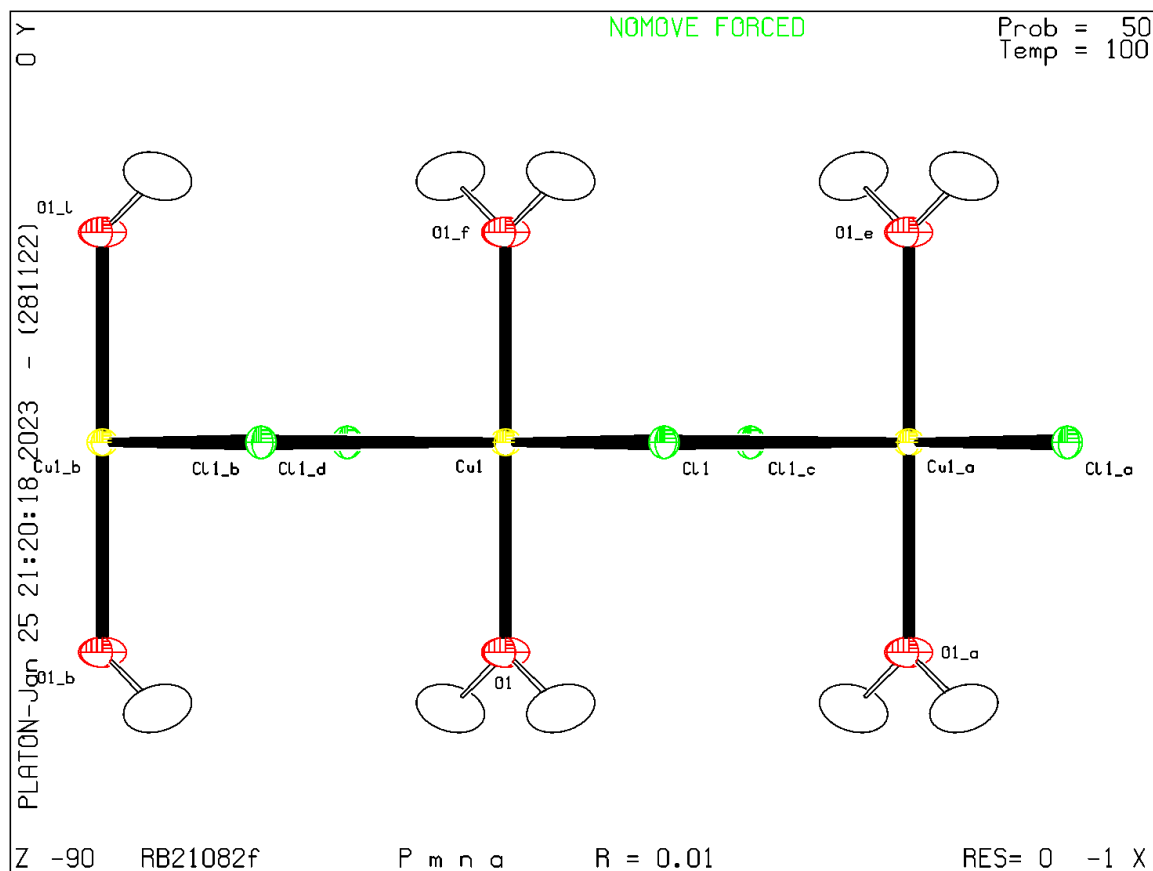
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.

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```
R(reflections)= 0.0133( 238)      wR2(reflections)=
S = 1.053                        0.0329( 238)
Npar= 26
```

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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 C**

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio .....	9.15	Note
PLAT742_ALERT_1_C	Angle Calc 90.00(1), Rep 90.00 .....		Missing s.u.
	O1 -CU1 -CL1 1_555 1_555 1_555 #	3	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3	Report

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#### **Alert level G**

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II) .	2.09	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	5	Note
PLAT940_ALERT_3_G	Fsqd Refinement With I > n * Sigma(I) Only .....		Please Check
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....		Please Check
PLAT979_ALERT_1_G	NoSpherA2 Scattering Factors Used .....		Please Note

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3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
7 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
0 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
3 ALERT type 5 Informative message, check

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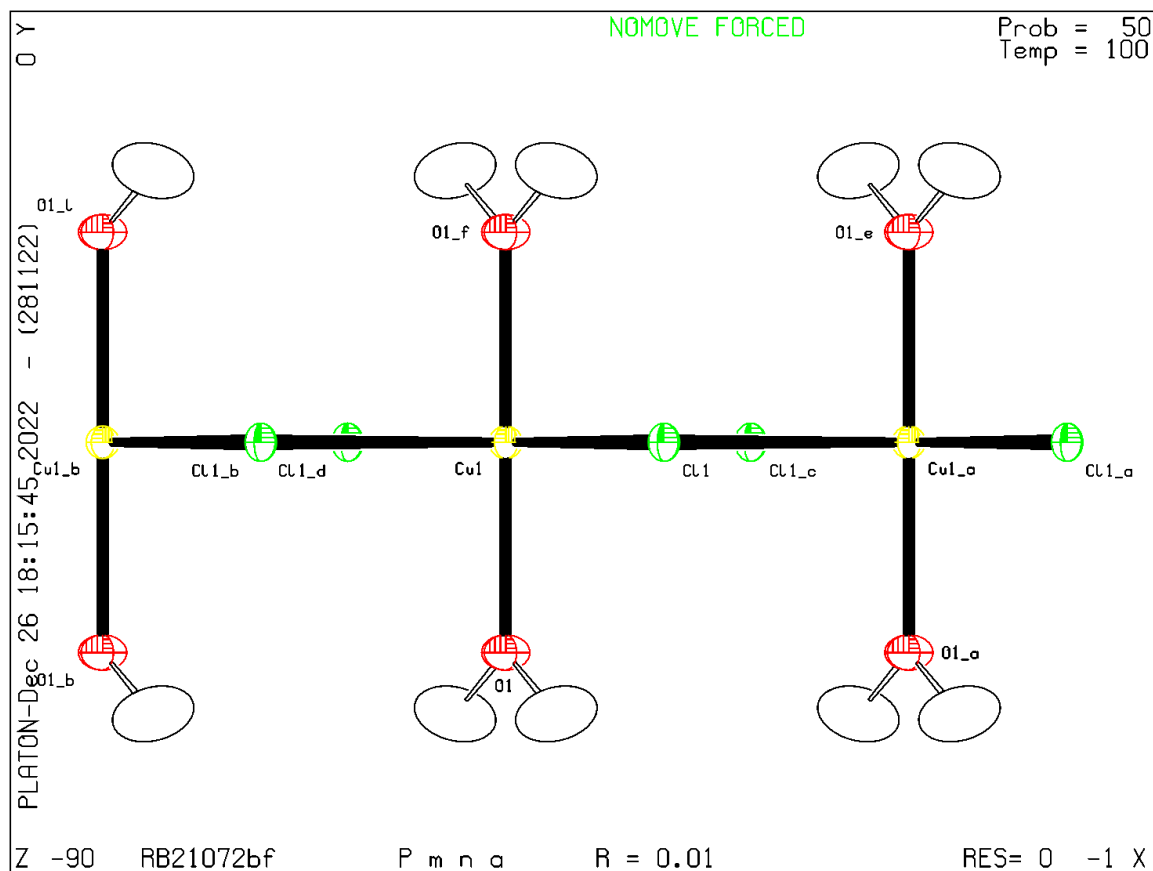
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## checkCIF/PLATON report

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No syntax errors found.      CIF dictionary      Interpreting this report

### Datablock: RB23004if

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Bond precision:	Ni- O = 0.0006 A	Wavelength=0.71073	
Cell:	a=6.5628 (4)	b=7.0330 (4)	c=8.7326 (6)
	alpha=90	beta=96.723 (6)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	400.29 (4)	400.29 (4)	
Space group	I 2/m	I 1 2/m 1	
Hall group	-I 2y	-I 2y	
Moiety formula	C12 H8 Ni O4, 2 (H2 O)	C12 H8 Ni O4, 2 (H2 O)	
Sum formula	C12 H12 Ni O6	C12 H12 Ni O6	
Mr	237.69	237.69	
Dx, g cm <sup>-3</sup>	1.972	1.972	
Z	2	2	
Mu (mm <sup>-1</sup> )	3.062	3.062	
F000	244.0	245.5	
F000'	245.39		
h, k, lmax	10, 11, 14	10, 11, 14	
Nref	997	890	
Tmin, Tmax	0.699, 0.912	0.762, 1.000	
Tmin'	0.571		

Correction method= # Reported T Limits: Tmin=0.762 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.893      Theta (max)= 35.720

R(reflections)= 0.0175 ( 838)	wR2(reflections)= 0.0400 ( 890)
S = 0.996	Npar= 56

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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 G**

PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1 Report
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 2 )	1.50 Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Ni (II) .	2.03 Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1 Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	108 Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....	Please Check
PLAT979_ALERT_1_G	NoSpherA2 Scattering Factors Used .....	Please Note

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0 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
4 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check
- 
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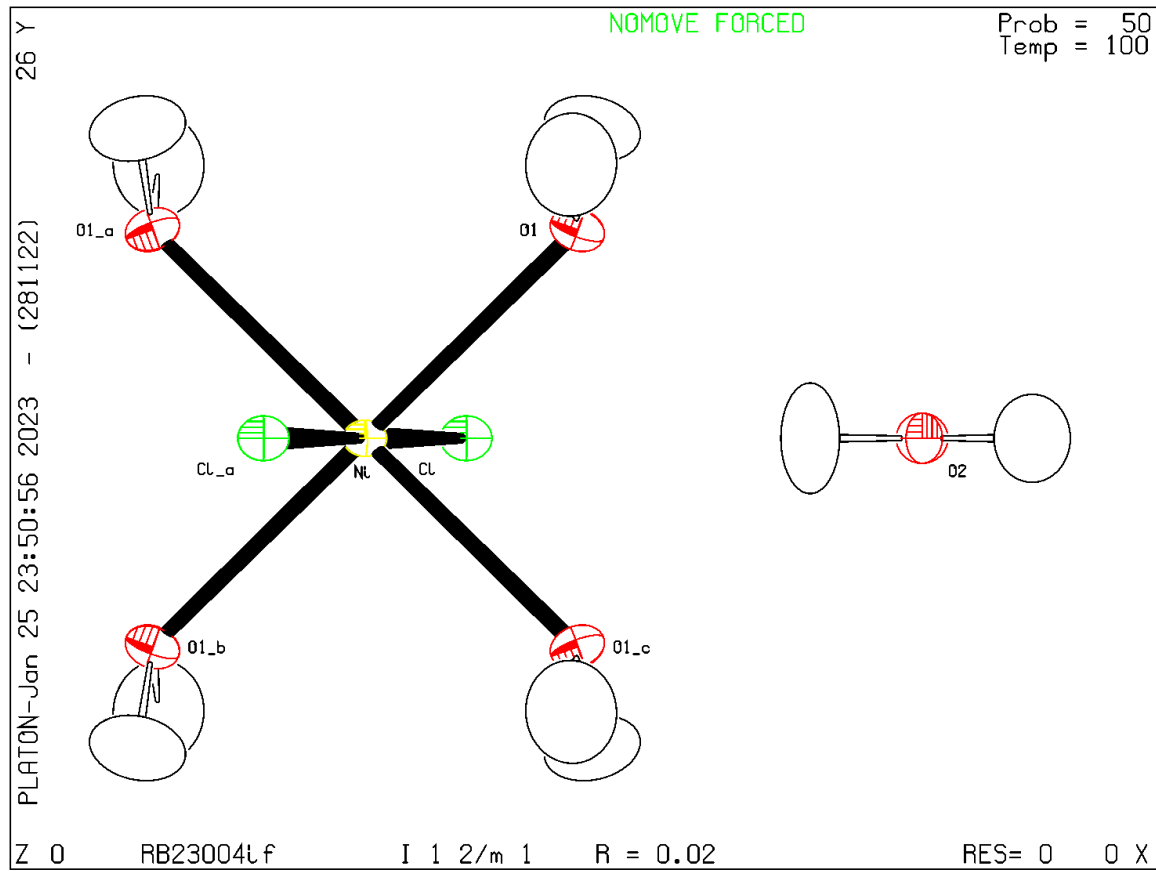
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No syntax errors found.      CIF dictionary      Interpreting this report

### Datablock: RB23005if

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Bond precision:	Ni- O = 0.0012 A	Wavelength=1.54184	
Cell:	a=6.5579 (2)	b=7.0244 (3)	c=8.7291 (3)
	alpha=90	beta=96.702 (4)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	399.36 (3)	399.36 (3)	
Space group	I 2/m	I 1 2/m 1	
Hall group	-I 2y	-I 2y	
Moiety formula	C12 H8 Ni O4, 2 (H2 O)	C12 H8 Ni O4, 2 (H2 O)	
Sum formula	C12 H12 Ni O6	C12 H12 Ni O6	
Mr	237.69	237.69	
Dx, g cm <sup>-3</sup>	1.977	1.977	
Z	2	2	
Mu (mm <sup>-1</sup> )	9.551	9.551	
F000	244.0	240.2	
F000'	240.05		
h, k, lmax	8, 8, 11	8, 8, 11	
Nref	474	469	
Tmin, Tmax	0.410, 0.682	0.382, 1.000	
Tmin'	0.097		

Correction method= # Reported T Limits: Tmin=0.382 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.989      Theta(max)= 80.170

R(reflections)= 0.0276 ( 447)	wR2(reflections)= 0.0843 ( 469)
S = 1.044	Npar= 56

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**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.

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#### **Alert level C**

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio .....	8.38	Note
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) O2 - H2A .	1.01	Ang.

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#### **Alert level G**

PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1 Report
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 2 )	1.50 Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Ni (II) .	2.04 Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	24 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	4 Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....	Please Check
PLAT979_ALERT_1_G	NoSpherA2 Scattering Factors Used .....	Please Note

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