

# checkCIF/PLATON report

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

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: CuCrO4-phen

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Bond precision:    C-C = 0.0440 A

Wavelength=1.54178

Cell:                a=5.6292(7)                b=5.6494(6)                c=13.7959(13)  
                      alpha=92.654(7)        beta=90.330(7)        gamma=109.093(8)  
Temperature:        293 K

	Calculated	Reported
Volume	414.05(8)	414.05(8)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C12 H8 Cr2 Cu3 N2 O10	C12 H8 Cr2 Cu3 N2 O10
Sum formula	C12 H8 Cr2 Cu3 N2 O10	C12 H8 Cr2 Cu3 N2 O10
Mr	634.85	634.82
Dx,g cm-3	2.546	2.546
Z	1	1
Mu (mm-1)	15.331	15.331
F000	309.0	309.0
F000'	303.55	
h,k,lmax	6,6,15	6,6,15
Nref	1190	1061
Tmin,Tmax	0.264,0.736	0.519,1.000
Tmin'	0.138	

Correction method= EMPIRICAL

Data completeness= 0.892

Theta(max)= 58.830

R(reflections)= 0.1997( 717)

wR2(reflections)= 0.5150( 1061)

S = 1.818

Npar= 143

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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

RFACR01\_ALERT\_3\_A The value of the weighted R factor is > 0.45

Weighted R factor given 0.515

PLAT029\_ALERT\_3\_A \_diffn\_measured\_fraction\_theta\_full Low ..... 0.891

PLAT084\_ALERT\_2\_A High wR2 Value ..... 0.51

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### Alert level B

REFLT03\_ALERT\_3\_B Reflection count < 90% complete (theta max?)  
From the CIF: \_diffrn\_reflms\_theta\_max 58.83  
From the CIF: \_diffrn\_reflms\_theta\_full 58.83  
From the CIF: \_reflms\_number\_total 1061  
TEST2: Reflms within \_diffrn\_reflms\_theta\_max  
Count of symmetry unique reflms 1190  
Completeness (\_total/calc) 89.16%

REFNR01\_ALERT\_3\_B Ratio of reflections to parameters is < 8 for a centrosymmetric structure  
sine(theta)/lambda 0.5550  
Proportion of unique data used 1.0000  
Ratio reflections to parameters 7.4196

RFACG01\_ALERT\_3\_B The value of the R factor is > 0.15  
R factor given 0.200

THETM01\_ALERT\_3\_B The value of sine(theta\_max)/wavelength is less than 0.575  
Calculated sin(theta\_max)/wavelength = 0.5550

PLAT031\_ALERT\_4\_B Refined Extinction Parameter within Range ..... 1.750 Sigma  
PLAT082\_ALERT\_2\_B High R1 Value ..... 0.20  
PLAT088\_ALERT\_3\_B Poor Data / Parameter Ratio ..... 7.42  
PLAT341\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.0440 Ang

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### Alert level C

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12  
Rint given 0.134

PLAT020\_ALERT\_3\_C The value of Rint is greater than 0.12 ..... 0.134

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference Cu1 -- O2 .. 0.16 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference Cu1 -- O5\_a .. 0.19 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference Cu2 -- O1 .. 0.18 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference Cr3 -- O3 .. 0.18 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference Cr3 -- O5 .. 0.16 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference N1 -- C1 .. 0.16 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference N1 -- C7 .. 0.18 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C2 -- C3 .. 0.19 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C4 -- C5 .. 0.18 Ang.

PLAT241\_ALERT\_2\_C Check High Ueq as Compared to Neighbors for C2  
PLAT241\_ALERT\_2\_C Check High Ueq as Compared to Neighbors for C5  
PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for N1  
PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for C4

PLAT366\_ALERT\_2\_C Short? C(sp?)-C(sp?) Bond C1 - C2 ... 1.39 Ang.  
PLAT366\_ALERT\_2\_C Short? C(sp?)-C(sp?) Bond C2 - C4 ... 1.39 Ang.  
PLAT366\_ALERT\_2\_C Short? C(sp?)-C(sp?) Bond C4 - C5 ... 1.39 Ang.

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### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 8  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained Atom Sites .... 13  
PLAT004\_ALERT\_5\_G Info: Polymeric Structure Found with Dimension . 3  
PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in the CIF ?  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large. 0.20  
PLAT093\_ALERT\_1\_G No su's on H-positions, refinement reported as . mixed  
PLAT199\_ALERT\_1\_G Check the Reported \_cell\_measurement\_temperature 293 K  
PLAT200\_ALERT\_1\_G Check the Reported \_diffrn\_ambient\_temperature 293 K  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Cu1 -- O3\_b .. 6.0 su  
PLAT301\_ALERT\_3\_G Note: Main Residue Disorder ..... 7 Perc.  
PLAT764\_ALERT\_4\_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.17 Ratio  
PLAT860\_ALERT\_3\_G Note: Number of Least-Squares Restraints ..... 86

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3 **ALERT level A** = Most likely a serious problem - resolve or explain

8 **ALERT level B** = A potentially serious problem, consider carefully  
18 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
12 **ALERT level G** = General information/check it is not something unexpected

3 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
13 **ALERT type 2** Indicator that the structure model may be wrong or deficient  
12 **ALERT type 3** Indicator that the structure quality may be low  
11 **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*, 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.

