

# checkCIF/PLATON report

No syntax errors found.    CIF dictionary    Interpreting this report

## Datablock: sw207

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Bond precision:    C-C = 0.0073 A                      Wavelength=1.54178

Cell:                      a=11.5633(3)              b=17.2944(4)              c=26.1148(7)  
                            alpha=90                      beta=92.536(2)              gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	5217.3(2)	5217.3(2)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C28 H20 Cr4 Cu2 O8 P12, 2(C16 Al F36 O4), 2(C H2 Cl2)	C28 H20 Cr4 Cu2 O8 P12, 2(C16 Al F36 O4), 2(C H2 Cl2)
Sum formula	C62 H24 Al2 Cl4 Cr4 Cu2 F72 O16 P12	C62 H24 Al2 Cl4 Cr4 Cu2 F72 O16 P12
Mr	3295.31	3295.31
Dx,g cm-3	2.098	2.098
Z	2	2
Mu (mm-1)	8.373	8.373
F000	3200.0	3200.0
F000'	3215.98	
h,k,lmax	13,20,31	13,20,31
Nref	9279	9157
Tmin,Tmax	0.127,0.396	0.176,0.396
Tmin'	0.041	

Correction method= ANALYTICAL

Data completeness= 0.987                      Theta(max)= 66.840

R(reflections)= 0.0537( 7805)              wR2(reflections)= 0.1563( 9157)

S = 1.103                                      Npar= 897

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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

PLAT220\_ALERT\_2\_A Large Non-Solvent    F              Ueq(max)/Ueq(min) ...              4.92 Ratio

**Author Response: This is a result of a strong thermal movement even at the low temperature of the measurement.**

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**Alert level B**

PLAT220\_ALERT\_2\_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.56 Ratio

**Author Response: This is a result of a strong thermal movement even at the low temperature of the measurement.**

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for F20A -- C25A .. 9.20 su  
PLAT232\_ALERT\_2\_B Hirshfeld Test Diff (M-X) Cu1 -- P4 .. 27.70 su  
PLAT232\_ALERT\_2\_B Hirshfeld Test Diff (M-X) Cu1 -- P5 .. 26.81 su  
PLAT242\_ALERT\_2\_B Check Low Ueq as Compared to Neighbors for C27A  
PLAT242\_ALERT\_2\_B Check Low Ueq as Compared to Neighbors for C27B  
PLAT431\_ALERT\_2\_B Short Inter HL..A Contact F35 .. F22B .. 2.52 Ang.  
PLAT432\_ALERT\_2\_B Short Inter X...Y Contact F34 .. C1SB .. 2.86 Ang.  
PLAT234\_ALERT\_4\_B Large Hirshfeld Difference F23A -- C26A .. 0.20 Ang.

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**Alert level C**

DIFMX01\_ALERT\_2\_C The maximum difference density is > 0.1\*ZMAX\*0.75  
\_refine\_diff\_density\_max given = 2.257  
Test value = 2.175  
DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75  
The relevant atom site should be identified.  
PLAT083\_ALERT\_2\_C SHELXL Second Parameter in WGHT unusually Large. 6.00  
PLAT097\_ALERT\_2\_C Maximum (Positive) Residual Density ..... 2.26 eA-3  
PLAT213\_ALERT\_2\_C Atom F27A has ADP max/min Ratio ..... 3.50 prola  
PLAT213\_ALERT\_2\_C Atom F31 has ADP max/min Ratio ..... 3.20 prola  
PLAT213\_ALERT\_2\_C Atom F34 has ADP max/min Ratio ..... 3.20 prola  
PLAT213\_ALERT\_2\_C Atom F35 has ADP max/min Ratio ..... 3.50 prola  
PLAT213\_ALERT\_2\_C Atom F36 has ADP max/min Ratio ..... 4.00 prola  
PLAT213\_ALERT\_2\_C Atom F19B has ADP max/min Ratio ..... 3.30 prola  
PLAT213\_ALERT\_2\_C Atom F20B has ADP max/min Ratio ..... 3.20 prola  
PLAT213\_ALERT\_2\_C Atom F26B has ADP max/min Ratio ..... 3.40 prola  
PLAT220\_ALERT\_2\_C Large Non-Solvent P Ueq(max)/Ueq(min) ... 2.64 Ratio

**Author Response: This is a result of a strong thermal movement even at the low temperature of the measurement.**

PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for F27A -- C27A .. 5.62 su  
PLAT232\_ALERT\_2\_C Hirshfeld Test Diff (M-X) Cu1 -- P1 .. 7.44 su  
PLAT232\_ALERT\_2\_C Hirshfeld Test Diff (M-X) Cu1 -- P3 .. 6.48 su  
PLAT232\_ALERT\_2\_C Hirshfeld Test Diff (M-X) Cr1 -- P2 .. 5.53 su  
PLAT232\_ALERT\_2\_C Hirshfeld Test Diff (M-X) Cr1 -- C6 .. 5.57 su  
PLAT232\_ALERT\_2\_C Hirshfeld Test Diff (M-X) Cr1 -- C7 .. 5.86 su  
PLAT241\_ALERT\_2\_C Check High Ueq as Compared to Neighbors for P6  
PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for Cr2  
PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for C18  
PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for C26A  
PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for C29  
PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for C30  
PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for C25B  
PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for C26B  
PLAT250\_ALERT\_2\_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.48

PLAT301_ALERT_3_C	Main Residue Disorder .....	10.00	Perc.
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds (x 1000) Ang ...	7	
PLAT431_ALERT_2_C	Short Inter HL..A Contact F9 .. O2 ..	2.87	Ang.
PLAT431_ALERT_2_C	Short Inter HL..A Contact F20A .. O3 ..	2.87	Ang.
PLAT431_ALERT_2_C	Short Inter HL..A Contact F36 .. O3 ..	2.81	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Cr2 -- C13 ..	0.12	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Cr2 -- C14 ..	0.11	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O2 -- C7 ..	0.10	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O3 -- C13 ..	0.10	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F17 -- C24 ..	0.12	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F21A -- C25A ..	0.13	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C18 -- C29 ..	0.11	Ang.
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors for	C1SB	
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3? Phosphorus.	P6	

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### ● Alert level G

ABSTM02\_ALERT\_3\_G The ratio of expected to reported Tmax/Tmin(RR) is > 1.10

Tmin and Tmax reported: 0.176 0.396

Tmin and Tmax expected: 0.132 0.396

RR = 1.332

Please check that your absorption correction is appropriate.

PLAT860\_ALERT\_3\_G Note: Number of Least-Squares Restraints ..... 42

PLAT302\_ALERT\_4\_G Anion/Solvent Disorder ..... 50.00 Perc.

PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 6

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1 **ALERT level A** = In general: serious problem

9 **ALERT level B** = Potentially serious problem

42 **ALERT level C** = Check and explain

4 **ALERT level G** = General alerts; check

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

39 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

12 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

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### 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.**

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**PLATON version of 12/11/2008; check.def file version of 12/11/2008**

