

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: sw163

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Bond precision:	C-C = 0.0123 Å	Wavelength=1.54178	
Cell:	a=21.3242(1)	b=26.9244(2)	c=33.3967(2)
	alpha=90	beta=90.508(1)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	19173.7(2)	19173.7(2)	
Space group	P 21/n	P 21/n	
Hall group	-P 2yn	-P 2yn	
	C90 H135 Cl10 Cu10 Fe9	C90 H135 Cl10 Cu10 Fe9	
Moiety formula	P45, Cl10 H15 Fe P5, 2(C7 H8)	P45, Cl10 H15 Fe P5, 2(C7 H8)	
	C114 H166 Cl10 Cu10 Fe10	C114 H166 Cl10 Cu10 Fe10	
Sum formula	P50	P50	
Mr	4633.47	4633.47	
Dx, g cm-3	1.605	1.605	
Z	4	4	
Mu (mm-1)	12.548	12.548	
F000	9280.0	9280.0	
F000'	9240.48		
h,k,lmax	24,30,38	24,30,38	
Nref	30306	28827	
Tmin,Tmax	0.164,0.222	0.127,0.222	
Tmin'	0.033		

Correction method= MULTI-SCAN

Data completeness= 0.951      Theta(max)= 62.150

R(reflections)= 0.0619( 22057)      wR2(reflections)= 0.1520( 28827)

S = 1.043      Npar= 1681

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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 B

THETM01\_ALERT\_3\_B The value of sine(theta\_max)/wavelength is less than 0.575  
Calculated sin(theta\_max)/wavelength = 0.5735

PLAT029_ALERT_3_B	_diffn_measured_fraction_theta_full	Low	.....	0.95
PLAT213_ALERT_2_B	Atom C1	has ADP max/min Ratio	.....	4.20 prola
PLAT213_ALERT_2_B	Atom C2	has ADP max/min Ratio	.....	4.20 prola
PLAT213_ALERT_2_B	Atom C3	has ADP max/min Ratio	.....	4.20 prola
PLAT213_ALERT_2_B	Atom C4	has ADP max/min Ratio	.....	4.20 prola
PLAT213_ALERT_2_B	Atom C5	has ADP max/min Ratio	.....	4.20 prola
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Cu3 -- P5	..	13.75 su
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Cu3 -- P7	..	12.34 su
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Cu3 -- P21	..	10.68 su
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Fe10 -- P46	..	13.86 su
PLAT242_ALERT_2_B	Check Low	Ueq as Compared to Neighbors for	Fe1B	

### Alert level C

PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	.....	14
PLAT213_ALERT_2_C	Atom C6	has ADP max/min Ratio	3.60 prola
PLAT213_ALERT_2_C	Atom C9	has ADP max/min Ratio	3.50 prola
PLAT213_ALERT_2_C	Atom C23	has ADP max/min Ratio	3.90 oblat
PLAT213_ALERT_2_C	Atom C52	has ADP max/min Ratio	3.40 prola
PLAT213_ALERT_2_C	Atom C53	has ADP max/min Ratio	3.20 prola
PLAT213_ALERT_2_C	Atom C63	has ADP max/min Ratio	3.60 oblat
PLAT213_ALERT_2_C	Atom C84	has ADP max/min Ratio	3.10 oblat
PLAT213_ALERT_2_C	Atom C88	has ADP max/min Ratio	3.10 oblat
PLAT220_ALERT_2_C	Large Non-Solvent	C Ueq(max)/Ueq(min)	3.21 Ratio
PLAT222_ALERT_3_C	Large Non-Solvent	H Ueq(max)/Ueq(min)	3.25 Ratio
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1 -- P6	6.64 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1 -- P11	5.80 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe1 -- C4	5.52 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe1 -- C5	6.61 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe10 -- P47	9.16 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe10 -- P48	9.88 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe10 -- P49	9.18 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe10 -- P50	5.58 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe10 -- C91	6.69 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe10 -- C95	5.21 su
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	....	2.47
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds (x 1000) Ang	...	12
PLAT432_ALERT_2_C	Short Inter X...Y Contact	C14 .. C64	3.20 Ang.
PLAT141_ALERT_4_C	su on a - Axis Small or Missing (x 100000)	.....	10 Ang.
PLAT142_ALERT_4_C	su on b - Axis Small or Missing (x 100000)	.....	20 Ang.
PLAT143_ALERT_4_C	su on c - Axis Small or Missing (x 100000)	.....	20 Ang.
PLAT380_ALERT_4_C	Check Incorrectly? Oriented X(sp2)-Methyl Moiety		C16
PLAT380_ALERT_4_C	Check Incorrectly? Oriented X(sp2)-Methyl Moiety		C18

### Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	220.40
PLAT301_ALERT_3_G	Note Main Residue Disorder	8.00 Perc.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	142
PLAT302_ALERT_4_G	Note Anion/Solvent Disorder	50.00 Perc.
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P18
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P19
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P23
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P24
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P28
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P29
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P32
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P33
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P34
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P37
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P38

PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P39
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P42
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P43
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P44
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	>P46
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	>P47
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	>P48
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	>P49
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	>P50
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	<P46B
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	<P47B
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	<P48B
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	<P49B
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	<P50B
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	!
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	9
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....	!

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0 **ALERT level A** = In general: serious problem  
 12 **ALERT level B** = Potentially serious problem  
 29 **ALERT level C** = Check and explain  
 32 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 32 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  
 33 ALERT type 4 Improvement, methodology, query or suggestion  
 1 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 19/05/2009; check.def file version of 13/05/2009

