

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw150II

Bond precision: C-C = 0.0057 A Wavelength=1.54178

Cell: a=15.7104(3) b=12.8337(4) c=19.6145(3)
 alpha=90 beta=107.871(2) gamma=90

Temperature: 123 K

	Calculated	Reported
Volume	3763.91(16)	3763.91(16)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C56 H54 Cu3 Mo2 N5 O4 P5, 3(B F4), 3(C H2 Cl2)	C56 H54 Cu3 Mo2 N5 O4 P5, 3(B F4), 3(C H2 Cl2)
Sum formula	C59 H60 B3 Cl6 Cu3 F12 Mo2 N5 O4 P5	C59 H60 B3 Cl6 Cu3 F12 Mo2 N5 O4 P5
Mr	1913.63	1913.63
Dx,g cm-3	1.689	1.689
Z	2	2
Mu (mm-1)	7.225	7.225
F000	1904.0	1904.0
F000'	1903.77	
h,k,lmax	18,15,23	18,15,23
Nref	7229[13791]	11524
Tmin,Tmax	0.085,0.285	0.139,0.434
Tmin'	0.018	

Correction method= ANALYTICAL

Data completeness= 1.59/0.84 Theta(max)= 68.260

R(reflections)= 0.0279(11471) wR2(reflections)= 0.0741(11524)

S = 1.054 Npar= 922

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.

Alert level B

PLAT222_ALERT_3_B	Large Non-Solvent	H	Ueq(max)/Ueq(min)	...	4.71	Ratio
PLAT230_ALERT_2_B	Hirshfeld Test Diff	for	O301	-- C301	..	8.41 su
PLAT232_ALERT_2_B	Hirshfeld Test Diff	(M-X)	Mo02	-- C301	..	10.97 su

● **Alert level C**

PLAT220_ALERT_2_C	Large Non-Solvent	C	Ueq(max)/Ueq(min)	...	3.84	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O400	--	C400	..	5.16 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo01	--	C400	..	7.40 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo01	--	C401	..	5.92 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo02	--	C300	..	5.70 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1	--	P4	..	6.78 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu2	--	N3	..	5.30 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu3	--	P5	..	8.11 su
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor				2.61
PLAT432_ALERT_2_C	Short Inter X...Y Contact	C1	..	F9B	..	2.93 Ang.
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of					B2
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of					B3

● **Alert level G**

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.

From the CIF: _diffrn_reflms_theta_max	68.26
From the CIF: _reflns_number_total	11524
Count of symmetry unique reflns	7229
Completeness (_total/calc)	159.41%
TEST3: Check Friedels for noncentro structure	
Estimate of Friedel pairs measured	4295
Fraction of Friedel pairs measured	0.594
Are heavy atom types Z>Si present	yes

PLAT301_ALERT_3_G	Note: Main Residue Disorder	4.00	Perc.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	31	
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder	11.00	Perc.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	10	
PLAT791_ALERT_4_G	The Model has Chirality at P2 (Verify)	R	

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 12 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
 - 6 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.

PLATON version of 13/08/2009; check.def file version of 12/08/2009

Datablock sw1501I - ellipsoid plot

