

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: chgr82

Bond precision: C-C = 0.0041 Å

Wavelength=0.71073

Cell: a=12.3323(8) b=17.8650(11) c=10.6673(7)

alpha=90

beta=109.439(1)

gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	2216.2(2)	2216.2(2)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C38 H60 B2 Cl2 Co2 N4 S4	?
Sum formula	C38 H60 B2 Cl2 Co2 N4 S4	C38 H60 B2 Cl2 Co2 N4 S4
Mr	911.56	911.52
Dx,g cm-3	1.366	1.366
Z	2	2
Mu (mm-1)	1.089	1.089
F000	956.0	956.0
F000'	959.15	
h,k,lmax	16,23,14	16,23,13
Nref	5489	4511
Tmin,Tmax	0.682,0.804	0.670,0.812
Tmin'	0.640	

Correction method= MULTI-SCAN

Data completeness= 0.822

Theta(max)= 28.250

R(reflections)= 0.0388(3841)

wR2(reflections)= 0.1127(4511)

S = 1.047

Npar= 235

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 A

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full Low 0.89

Author Response: Crystals consistently weak diffractors. The data herein represent the best of several trials.



Alert level C

PLAT222_ALERT_3_C	Large Non-Solvent	H	Ueq(max)/Ueq(min) ...	3.10	Ratio
PLAT242_ALERT_2_C	Check Low		Ueq as Compared to Neighbors for	C4	
PLAT194_ALERT_1_C	Missing _cell_measurement_reflms_used		datum	?	
PLAT195_ALERT_1_C	Missing _cell_measurement_theta_max		datum	?	
PLAT196_ALERT_1_C	Missing _cell_measurement_theta_min		datum	?	

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

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

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

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

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

1 **ALERT type 2** Indicator that the structure model may be wrong or deficient

2 **ALERT type 3** Indicator that the structure quality may be low

0 **ALERT type 4** Improvement, methodology, query or suggestion

0 **ALERT type 5** Informative message, check

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

