

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: jml45

Bond precision: C-C = 0.0113 A

Wavelength=0.71073

Cell: a=13.8646(10) b=14.0687(12) c=14.3634(10)
alpha=99.049(6) beta=118.343(6) gamma=106.634(6)
Temperature: 200 K

	Calculated	Reported
Volume	2215.3(4)	2215.2(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C76 H94 Mn6 N12 O22, 2(C H Cl3)	C76 H94 Mn6 N12 O22, 2(C H Cl3)
Sum formula	C78 H96 Cl6 Mn6 N12 O22	C78 H96 Cl6 Mn6 N12 O22
Mr	2096.01	2096.01
Dx,g cm-3	1.571	1.571
Z	1	1
Mu (mm-1)	1.088	1.088
F000	1076.0	1076.0
F000'	1079.30	
h,k,lmax	18,18,18	18,18,18
Nref	10172	10108
Tmin,Tmax	0.866,0.917	0.613,0.917
Tmin'	0.813	

Correction method= MULTI-SCAN

Data completeness= 0.994

Theta(max)= 27.500

R(reflections)= 0.0725(5800)

wR2(reflections)= 0.2130(10108)

S = 1.036

Npar= 567

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

PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 4.23 Ratio



Alert level C

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 11

PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C28 - C29 ... 1.42 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C28 -- C29 .. 0.18 Ang.
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C39

● **Alert level G**

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.11
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 1
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal (x 10000) 600 Deg.

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
2 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 29/06/2010; check.def file version of 26/06/2010

