checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: jml35b

Bond precision: C-C = 0.0059 A   Wavelength=0.71073

Cell: a=13.370(2)   b=14.8788(15)   c=15.747(2)
               alpha=111.536(10) beta=106.607(17) gamma=102.280(11)
Temperature: 200 K

	Calculated	Reported
Volume	2609.1(8)	2609.0(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C92 H126 Mn6 N12 O22	C92 H126 Mn6 N12 O22
Sum formula	C92 H126 Mn6 N12 O22	C92 H126 Mn6 N12 O22
Mr	2081.69	2081.69
Dx,g cm-3	1.325	1.325
Z	1	1
Mu (mm-1)	0.774	0.774
F000	1088.0	1088.0
F000'	1090.44	
h,k,lmax	18,20,22	18,20,22
Nref	15201	15034
Tmin,Tmax	0.830,0.940	0.706,0.940
Tmin'	0.734	

Correction method= MULTI-SCAN

Data completeness= 0.989   Theta(max)= 30.000

R(reflections)= 0.0480(7805)   wR2(reflections)= 0.1484(15034)

S = 1.000   Npar= 632

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) ...   4.17 Ratio
PLAT241_ALERT_2_B Check High   Ueq as Compared to Neighbors for   C22
PLAT242_ALERT_2_B Check Low   Ueq as Compared to Neighbors for   C21A
PLAT242_ALERT_2_B Check Low   Ueq as Compared to Neighbors for   C21B

Alert level C

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....        3.45
PLAT222_ALERT_3_C Large Non-Solvent    H     Ueq(max)/Ueq(min) ...        3.61 Ratio
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C37
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C19A
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C41
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C44
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C19B
```

Alert level G

```
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................        4.00 Perc.
PLAT333_ALERT_2_G Check Large Av C6-Ring C-C Dist. C23     -C28           1.41 Ang.
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....        0.40 mm
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......       28.10 Deg.
          H22C -C22  -H22F    1.555    1.555    1.555
```

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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 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 06/08/2009; check.def file version of 04/08/2009

NOMOVE FORCED

Prob = 50
Temp = 200

49 Y

PLATON-Aug 10 15:10:17 2009 - (60809)

Z -168   jml35b   P -1   R = 0.05   RES=   0   -60 X