checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: jml51

Bond precision: C-C = 0.0053 A Wavelength=0.71073

Cell: a=14.2679(17) b=22.150(3) c=16.5298(14)
alpha=90 beta=115.124(8) gamma=90
Temperature: 200 K

	Calculated	Reported
Volume	4729.7(10)	4729.8(9)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C88 H118 Mn6 N12 O22	C88 H118 Mn6 N12 O22
Sum formula	C88 H118 Mn6 N12 O22	C88 H118 Mn6 N12 O22
Mr	2025.59	2025.58
Dx,g cm-3	1.422	1.422
Z	2	2
Mu (mm-1)	0.852	0.852
F000	2112.0	2112.0
F000’	2116.85	
h,k,lmax	20,31,23	20,31,23
Nref	13788	13721
Tmin,Tmax	0.799,0.829	0.562,0.894
Tmin’	0.795	

Correction method= MULTI-SCAN

Data completeness= 0.995 Theta(max)= 30.000

R(reflections)= 0.0457(7986) wR2(reflections)= 0.1387(13721)

S = 1.010 Npar= 647

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) ... 4.81 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for N6 -- C33 .. 10.06 su
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C44A
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for N4B
PLAT245_ALERT_2_B U(iso) H44A Smaller than U(eq) C45B by ... 0.08 AngSq
PLAT410_ALERT_2_B Short Intra H...H Contact H17 .. H20D .. 1.81 Ang.

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PLAT413_ALERT_2_B Short Inter XH3 .. XHn     H41    ..  H23E    ..       2.08 Ang.
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Alert level C

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PLAT215_ALERT_3_C Disordered C44B      has ADP max/min Ratio .....       3.50
PLAT215_ALERT_3_C Disordered C45B      has ADP max/min Ratio .....       3.20
PLAT222_ALERT_3_C Large Non-Solvent    H     Uiso(max)/Uso(min) ...       4.52 Rati
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C33    --  C34     ..       5.13 su
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C40
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        O11
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        N4A
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C20A
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C35
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C45A
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C20B
PLAT245_ALERT_2_C U(iso) H44B    Smaller than U(eq) C44B    by ...       0.05 AngSq
PLAT245_ALERT_2_C U(iso) H45A    Smaller than U(eq) C45B    by ...       0.02 AngSq
PLAT245_ALERT_2_C U(iso) H45B    Smaller than U(eq) C45B    by ...       0.02 AngSq
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C33    -   C34    ...       1.41 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N4A    --  C20A    ..       0.15 Ang.
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Alert level G

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PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................      10.00 Perc.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         10
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c   .......      P21/n
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      21.70 Deg.
              C44B -O11  -C44A    1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF ......      37.00 Deg.
              N4B  -C19  -N4A     1.555   1.555   1.555
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   0 ALERT level A = In general: serious problem
   7 ALERT level B = Potentially serious problem
  16 ALERT level C = Check and explain
   5 ALERT level G = General alerts; check

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  19 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   4 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 29/06/2010; check.def file version of 26/06/2010

Datablock jml51 - ellipsoid plot