

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: MnY

Bond precision: C-C = 0.0058 A

Wavelength=0.71073

Cell: a=13.1987(7) b=13.5750(8) c=14.1952(7)
 alpha=71.486(5) beta=64.349(5) gamma=81.392(4)
Temperature: 156 K

	Calculated	Reported
Volume	2173.9(2)	2173.8(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C50 H90 Mn2 O22 Y2, 2(C6 H15 N), 3(C2 N)	C50 H90 Mn2 O22 Y2, 2(C6 H15 N), 3(C2 N)
Sum formula	C68 H120 Mn2 N5 O22 Y2	C68 H120 Mn2 N5 O22 Y2
Mr	1647.39	1647.38
Dx,g cm-3	1.258	1.258
Z	1	1
Mu (mm-1)	1.670	1.670
F000	867.0	867.0
F000'	862.45	
h,k,lmax	17,18,19	16,18,19
Nref	11424	9805
Tmin,Tmax	0.869,0.905	0.767,1.000
Tmin'	0.846	

Correction method= # Reported T Limits: Tmin=0.767 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.858

Theta(max)= 28.859

R(reflections)= 0.0434(7813)

wR2(reflections)= 0.1162(9805)

S = 1.028

Npar= 612

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 C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.51	Report
PLAT213_ALERT_2_C	Atom O1B has ADP max/min Ratio	3.3	prolat
PLAT220_ALERT_2_C	Large Non-Solvent C Ueq(max)/Ueq(min) Range	3.8	Ratio
PLAT220_ALERT_2_C	Large Non-Solvent O Ueq(max)/Ueq(min) Range	5.0	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C28B -- C29B ..	0.16	Ang.
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	03	Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	09	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	C7	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	C12	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	N2	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	3.8	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.5	Note



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	29	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Y1 -- O4 ..	8.1	su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Y1 -- O10 ..	5.9	su
PLAT300_ALERT_4_G	Atom Site Occupancy of >O1B is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <O2 is Constrained at	0.424	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C1B is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C3 is Constrained at	0.710	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C4 is Constrained at	0.710	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C5 is Constrained at	0.710	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1 is Constrained at	0.424	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C3B is Constrained at	0.290	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C4B is Constrained at	0.290	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C5B is Constrained at	0.290	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >O1B_a is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <O2_a is Constrained at	0.424	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C1B_a is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C3_a is Constrained at	0.710	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C4_a is Constrained at	0.710	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C5_a is Constrained at	0.710	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C1_a is Constrained at	0.424	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C3B_a is Constrained at	0.290	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C4B_a is Constrained at	0.290	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C5B_a is Constrained at	0.290	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >N1B is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C26B is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C27B is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C28B is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C29B is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C30B is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C31B is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <N1 is Constrained at	0.424	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C26 is Constrained at	0.424	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C27 is Constrained at	0.424	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C28 is Constrained at	0.424	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C29 is Constrained at	0.424	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C30 is Constrained at	0.424	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C31 is Constrained at	0.424	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C32B is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C33B is Constrained at	0.576	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C32 is Constrained at	0.424	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of <C33	is Constrained at	0.424	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *N3	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C1A	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C2	is Constrained at	0.500	Check
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage =	13	Note
PLAT302_ALERT_4_G	Anion/Solvent Disorder	Percentage =	91	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (12.67) in Resd. #		2	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (9.33) in Resd. #		3	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (1.50) in Resd. #		5	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact N3 .. C2 ..		1.46	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact N3 .. C32B ..		2.36	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact N3 .. C1A ..		2.68	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1A .. C2 ..		1.04	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1A .. C1A ..		1.71	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1A .. C32B ..		2.39	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C2 .. C2 ..		1.86	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C2 .. C27B ..		2.69	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C2 .. C32B ..		3.08	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		11	Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .		1.24	Ratio
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C1A -- C1A .		1.71	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C2 -- C2 .		1.86	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		199	Check
	C2 -C1A -C1A 1.555 1.555 2.773		37.30	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		205	Check
	C1A -C2 -C2 1.555 1.555 2.773		33.70	Deg.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	C6 H15 N			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		3	Note
	C6 H15 N			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		4	Note
	C2 N			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		5	Note
	C2 N			
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		135	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 70 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 24 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
 55 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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.

