

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: 3

Bond precision:	C-C = 0.0076 A	Wavelength=1.54178
Cell:	a=19.0904 (1)	b=26.7042 (2) c=24.9905 (2)
	alpha=90	beta=92.444 (1) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	12728.42 (15)	12728.42 (15)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C135 H85 N O26 Y4 [+ solvent]	?
Sum formula	C135 H85 N O26 Y4 [+ solvent]	C135 H95 N O29 Y4
Mr	2492.69	2550.72
Dx, g cm-3	1.301	1.329
Z	4	4
Mu (mm-1)	2.937	2.966
F000	5064.0	5184.0
F000'	5073.97	
h, k, lmax	24, 33, 31	24, 32, 30
Nref	26768	25643
Tmin, Tmax	0.515, 0.743	0.478, 1.000
Tmin'	0.291	

Correction method= # Reported T Limits: Tmin=0.478 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.958

Theta(max)= 76.512

R(reflections)= 0.0581(23363)

wR2(reflections)=
0.1788(25643)

S = 1.091

Npar= 1495

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

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C31	--C32	.	7.3 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	C43	--C44	.	8.5 s.u.
PLAT415_ALERT_2_B	Short Inter D-H..H-X	H6	..H7A	.	1.99 Ang.
			-x,1-y,1-z =		3_566 Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O7	--H7A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O26	--H26B	.	Please Check



Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.74 Report

PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 3.02 eA-3

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio

PLAT230_ALERT_2_C Hirshfeld Test Diff for O18 --C121 . 5.5 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C32 --C33 . 6.3 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C33 --C38 . 6.0 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C38 --C39 . 7.0 s.u.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C43 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C44 Check

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00757 Ang.

PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C31 - C32 . 1.53 Ang.

PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C40 - C45 . 1.53 Ang.



Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum: C135 H95 N1 O29 Y4
Atom count from the _atom_site data: C135 H85 N1 O26 Y4

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C135 H95 N O29 Y4
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	540.00	540.00	0.00
H	380.00	340.00	40.00
N	4.00	4.00	0.00

O	116.00	104.00	12.00	
Y	16.00	16.00	0.00	

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 135 Report
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report
 PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
 PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 20.93 Why ?
 PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing 0.00020 Ang.
 PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing 0.00020 Ang.
 PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
 PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report
 PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
 PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
 PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Y4 --O10 . 6.0 s.u.
 PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C2 -C7 0.15 Ang.
 PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C32 -C45 0.24 Ang.
 PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C33 -C38 0.16 Ang.
 PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C40 -C45 0.19 Ang.
 PLAT432_ALERT_2_G Short Inter X...Y Contact C84 ..C86 . 3.19 Ang.
 -x,2-y,1-z = 3_576 Check
 PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Y1 (III) . 3.13 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Y2 (III) . 3.32 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Y3 (III) . 3.35 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Y4 (III) . 3.39 Info
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 3582 Note
 PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
 PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.7 Low
 PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check

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

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 26 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
 5 ALERT type 4 Improvement, methodology, query or suggestion
 5 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* or *IUCrData*, 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.

