

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: 3a

Bond precision:	C-C = 0.0065 A	Wavelength=1.54178
Cell:	a=19.1701 (1)	b=26.5636 (1) c=24.8806 (1)
	alpha=90	beta=92.300 (1) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	12659.66 (10)	12659.66 (10)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C270 H168 N2 O52 Y8 [+ solvent]	?
Sum formula	C270 H168 N2 O52 Y8 [+ solvent]	C270 H184 N2 O55 Y8
Mr	4983.36	5047.40
Dx, g cm ⁻³	1.307	1.322
Z	2	2
Mu (mm ⁻¹)	2.953	2.968
F000	5060.0	5124.0
F000'	5069.97	
h, k, lmax	24, 33, 31	24, 33, 31
Nref	27133	25869
Tmin, Tmax	0.515, 0.743	0.189, 1.000
Tmin'	0.291	

Correction method= # Reported T Limits: Tmin=0.189 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.953

Theta(max)= 78.123

R(reflections)= 0.0485(23125)

wR2(reflections)=
0.1417(25869)

S = 1.063

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

PLAT094_ALERT_2_B	Ratio of Maximum / Minimum Residual Density	4.01	Report
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O7 --H7A .		Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor O22 --H22B .		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.

PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	3.43	eA-3
PLAT213_ALERT_2_C	Atom C66 has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C	Atom C67 has ADP max/min Ratio	3.7	prolat
PLAT213_ALERT_2_C	Atom C69 has ADP max/min Ratio	3.3	prolat
PLAT213_ALERT_2_C	Atom C71 has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C	Atom C72 has ADP max/min Ratio	3.3	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	5.7	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.4	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C4 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C50 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C66 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C67 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C69 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C72 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C127 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C129 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C68 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C70 Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0065	Ang.
PLAT414_ALERT_2_C	Short Intra D-H..H-X H7A ..H94 .	1.91	Ang.
	x,y,z =	1_555	Check

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: C270 H184 N2 O55 Y8

Atom count from the _atom_site data: C270 H168 N2 O52 Y8

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 2

From the CIF: _chemical_formula_sum C270 H184 N2 O55 Y8

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff	
C	540.00	540.00	0.00	
H	368.00	336.00	32.00	
N	4.00	4.00	0.00	
O	110.00	104.00	6.00	
Y	16.00	16.00	0.00	

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	15.20	Why ?
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing	0.00010	Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing	0.00010	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C63 -C68	0.20	Ang.
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C8	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1 - C8_a	1.64	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C7 - C8	1.51	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C8 - C9	1.50	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C39 ..C41	3.16	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)	3.09	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Y2 (III)	3.19	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Y3 (III)	3.32	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Y4 (III)	3.38	Info
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
 3 **ALERT level B** = A potentially serious problem, consider carefully
 22 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 25 **ALERT level G** = General information/check it is not something unexpected

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 30 ALERT type 2 Indicator that the structure model may be wrong or deficient
 3 ALERT type 3 Indicator that the structure quality may be low
 4 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.

