

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: 3m

Bond precision:	C-C = 0.0147 A	Wavelength=0.71073
Cell:	a=19.1796 (7)	b=26.7579 (11) c=24.9832 (8)
	alpha=90	beta=92.183 (3) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	12812.2 (8)	12812.2 (8)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C135 H84 N O26 Y4 [+ solvent]	?
Sum formula	C135 H84 N O26 Y4 [+ solvent]	C135 H95 N O29 Y4
Mr	2491.68	2550.75
Dx, g cm ⁻³	1.292	1.322
Z	4	4
Mu (mm ⁻¹)	1.863	1.866
F000	5060.0	5200.0
F000'	5017.58	
h, k, lmax	22, 31, 29	22, 31, 29
Nref	22605	22595
Tmin, Tmax	0.645, 0.830	0.701, 1.000
Tmin'	0.469	

Correction method= # Reported T Limits: Tmin=0.701 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.000

Theta(max)= 25.009

R(reflections)= 0.0748(13169)

wR2(reflections)=
0.2467(22595)

S = 1.016

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

PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	C125	Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O18	--H18A	.	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

PLAT213_ALERT_2_C	Atom C101	has ADP max/min Ratio		3.2	oblate
PLAT220_ALERT_2_C	NonSolvent	Resd 1 C	Ueq(max)/Ueq(min) Range	3.4	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C6	--C7	.	5.8 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C12	--C13	.	5.8 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C32	--C45	.	7.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C38	--C39	.	6.7 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C121	--C122	.	5.1 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C123	--C124	.	6.4 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C125	--C126	.	5.2 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C127	--C128	.	6.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C129	--C130	.	5.7 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C134	--C135	.	5.8 s.u.
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Y4	--O9	.	5.7 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C2	--C3	.	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C3	--C4	.	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C8	--C9	.	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C10	--C11	.	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C18	--C19	.	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C24	--C25	.	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C26	--C27	.	0.24 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C29	--C30	.	0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C33	--C34	.	0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C40	--C41	.	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C41	--C42	.	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C43	--C44	.	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C44	--C45	.	0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C48	--C49	.	0.22 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C48	--C53	.	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C69	--C70	.	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C71	--C72	.	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C73	--C74	.	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C80	--C81	.	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C83	--C84	.	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C85	--C86	.	0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C93	--C98	.	0.18 Ang.

PLAT234_ALERT_4_C	Large	Hirshfeld	Difference	C94	--C95	.	0.18	Ang.
PLAT234_ALERT_4_C	Large	Hirshfeld	Difference	C97	--C98	.	0.18	Ang.
PLAT234_ALERT_4_C	Large	Hirshfeld	Difference	C98	--C99	.	0.16	Ang.
PLAT234_ALERT_4_C	Large	Hirshfeld	Difference	C99	--C100	.	0.18	Ang.
PLAT234_ALERT_4_C	Large	Hirshfeld	Difference	C103	--C104	.	0.18	Ang.
PLAT234_ALERT_4_C	Large	Hirshfeld	Difference	C110	--C111	.	0.16	Ang.
PLAT234_ALERT_4_C	Large	Hirshfeld	Difference	C115	--C120	.	0.16	Ang.
PLAT234_ALERT_4_C	Large	Hirshfeld	Difference	C123	--C128	.	0.19	Ang.
PLAT234_ALERT_4_C	Large	Hirshfeld	Difference	C124	--C125	.	0.23	Ang.
PLAT234_ALERT_4_C	Large	Hirshfeld	Difference	C130	--C135	.	0.18	Ang.
PLAT234_ALERT_4_C	Large	Hirshfeld	Difference	C133	--C134	.	0.25	Ang.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			03	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			05	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			06	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			011	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			015	Check
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			C6	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C8	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C11	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C12	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C21	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C27	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C39	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C42	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C52	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C54	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C56	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C57	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C71	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C80	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C88	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C95	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C99	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C101	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C102	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C123	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			C132	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of			C133	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			Y2	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			Y3	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			C9	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			C10	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			C14	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			C40	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			C60	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			C100	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			C124	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			C126	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			C128	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			C131	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of			C135	Check
PLAT260_ALERT_2_C	Large	Average	Ueq of Residue Including		Y1		0.103	Check
PLAT341_ALERT_3_C	Low	Bond Precision on	C-C Bonds				0.01471	Ang.
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond	C2	- C7	.		1.53	Ang.
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond	C61	- C62	.		1.54	Ang.

PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C121 - C122 . 1.55 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 H84 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	336.00	44.00
N	4.00	4.00	0.00
O	116.00	104.00	12.00
Y	16.00	16.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	24	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	29	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
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	11	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	6	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	2	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar	0.0200	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar	0.0200	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar	0.0200	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar	0.0200	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar	0.0200	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar	0.0200	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0400	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar	0.0200	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C48 -C53 .	1.42	Ang.
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C93 -C98 .	1.43	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C2 -C7	0.21	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C9 -C14	0.21	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C25 -C30	0.16	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C47 -C60	0.17	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C92 -C105	0.19	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C93 -C98	0.16	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C115 -C120	0.16	Ang.
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C1	Check
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 - C15 .	1.59	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C8 .	2.97	Ang.
	1-x,2-y,-z =	3_675	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C8 .	1.95	Ang.
	1-x,2-y,-z =	3_675	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C9 .	2.72	Ang.
	1-x,2-y,-z =	3_675	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C7 .	2.79	Ang.
	1-x,2-y,-z =	3_675	Check

PLAT432_ALERT_2_G Short Inter X...Y Contact	C2	..C8	.	2.78 Ang.
		1-x,2-y,-z =		3_675 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2	..C9	.	2.85 Ang.
		1-x,2-y,-z =		3_675 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C7	..C14	.	2.87 Ang.
		1-x,2-y,-z =		3_675 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C7	..C9	.	3.09 Ang.
		1-x,2-y,-z =		3_675 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C8	..C14	.	2.70 Ang.
		1-x,2-y,-z =		3_675 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C8	..C15	.	2.84 Ang.
		1-x,2-y,-z =		3_675 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C8	..C8	.	3.16 Ang.
		1-x,2-y,-z =		3_675 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C69	..C71	.	3.18 Ang.
		1-x,1-y,-z =		3_665 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure				! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Y1	(III)	.		3.41 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Y2	(III)	.		3.19 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Y3	(III)	.		3.09 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Y4	(III)	.		3.30 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints				174 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
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..				50.0 Degree

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 89 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 ALERT type 3 Indicator that the structure quality may be low
 38 ALERT type 4 Improvement, methodology, query or suggestion
 6 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.

