

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: 123

Bond precision: C-C = 0.0241 Å Wavelength=0.71069

Cell: a=19.366(5) b=19.366(5) c=18.436(5)
 alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	6914(4)	6914(3)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C150 H104 O25 Yb5, C2 Cl4, 2(C Cl2)	C150 H104 O25 Yb5, C2 Cl4, 2(C Cl2)
Sum formula	C154 H104 Cl8 O25 Yb5	C154 H104 Cl8 O25 Yb5
Mr	3503.17	3503.17
Dx, g cm ⁻³	1.683	1.683
Z	2	2
Mu (mm ⁻¹)	3.575	3.575
F000	3428.0	3428.0
F000'	3427.93	
h,k,lmax	23,23,21	23,23,21
Nref	6100	6100
Tmin,Tmax	0.422,0.628	0.422,0.628
Tmin'	0.329	

Correction method= MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.000

R(reflections)= 0.0541(4558) wR2(reflections)= 0.1421(6100)

S = 1.122 Npar= 427

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

PLAT213_ALERT_2_B	Atom C12	has ADP max/min Ratio	4.6	oblate
PLAT213_ALERT_2_B	Atom C36	has ADP max/min Ratio	4.7	prolat
PLAT213_ALERT_2_B	Atom C37	has ADP max/min Ratio	5.0	prolat
PLAT220_ALERT_2_B	Large Non-Solvent C	Ueq(max)/Ueq(min) Range	10.0	Ratio
PLAT222_ALERT_3_B	Large Non-Solvent H	Uiso(max)/Uiso(min) ..	8.6	Ratio
PLAT241_ALERT_2_B	High	Ueq as Compared to Neighbors for	C16	Check
PLAT241_ALERT_2_B	High	Ueq as Compared to Neighbors for	C36	Check
PLAT242_ALERT_2_B	Low	Ueq as Compared to Neighbors for	C14	Check
PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds		0.0241	Ang.
PLAT369_ALERT_2_B	Long C(sp2)-C(sp2) Bond C14 - C16 ...		1.57	Ang.

● Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density		3.03	Report
PLAT147_ALERT_1_C	su on Symmetry Constrained Cell Angle(s)			Please Check
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent		2	
PLAT213_ALERT_2_C	Atom C13	has ADP max/min Ratio	3.4	prolat
PLAT213_ALERT_2_C	Atom C20	has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C	Atom C21	has ADP max/min Ratio	3.9	prolat
PLAT213_ALERT_2_C	Atom C35	has ADP max/min Ratio	3.6	prolat
PLAT221_ALERT_2_C	Large Solv./Anion C1	Ueq(max)/Ueq(min) Range	4.8	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C14 -- C38 ..		6.1	su
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C13	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C21	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C30	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C31	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C35	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	05	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C12	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C17	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C18	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C38	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		C98	Check
PLAT368_ALERT_2_C	Short C(sp2)-C(sp2) Bond C12 - C37 ...		1.18	Ang.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		3	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		8	Report
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF			Please Do !
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.		98.75	Why ?
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as .			mixed
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	(K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	(K)	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage =	1	Note
PLAT302_ALERT_4_G	Anion/Solvent Disorder	Percentage =	47	Note
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C38	Che
PLAT432_ALERT_2_G	Short Inter X...Y Contact C11 .. C97 ..		2.96	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C12 .. C97 ..		2.45	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C12 .. C42 ..		3.25	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C21 .. C98 ..		3.05	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C97 .. C97 ..		3.12	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C97 .. C97 ..		3.12	Ang.
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .		1.14	Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		196	Check
	C97 -CL1 -CL2 1.555 1.555 1.555		29.00	Deg.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	C2 C14			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		3	Note
	C C12			

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 36 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
 7 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.

