

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: 2

Bond precision:	C-C = 0.0060 A	Wavelength=1.54184
Cell:	a=13.3943 (1)	b=15.5141 (1) c=23.9524 (2)
	alpha=90	beta=91.861 (1) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	4974.70 (6)	4974.70 (6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C32 H68 Cl4 Mg O4 Si4 Th, C4 H8 O	C32 H68 Cl4 Mg O4 Si4 Th, C4 H8 O
Sum formula	C36 H76 Cl4 Mg O5 Si4 Th	C36 H76 Cl4 Mg O5 Si4 Th
Mr	1099.48	1099.47
Dx, g cm ⁻³	1.468	1.468
Z	4	4
Mu (mm ⁻¹)	12.966	12.966
F000	2232.0	2232.0
F000'	2230.28	
h, k, lmax	16, 18, 28	16, 18, 28
Nref	9101	8983
Tmin, Tmax	0.085, 0.354	0.206, 1.000
Tmin'	0.011	

Correction method= # Reported T Limits: Tmin=0.206 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.987 Theta(max)= 68.161

R(reflections)= 0.0239 (8764)	wR2(reflections)= 0.0639 (8983)
S = 1.028	Npar= 502

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**

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C018	Check	
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C01B	Check	
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C16	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C019	Check	
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	C20	Check	
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond	C015 - C01B	1.41	Ang.	

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	3	Report
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	0.00020	Ang.
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Th1 --Cl1	5.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Th1 --Cl2	12.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Th1 --Cl3	8.8	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Th1 --Cl4	6.3	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	4%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	20%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	25	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	14	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.1	Low

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 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
8 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

