

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: 5

Bond precision:	C-C = 0.0182 Å	Wavelength=1.54184	
Cell:	a=13.3309 (2) alpha=90	b=17.7676 (2) beta=90.681 (1)	c=33.4350 (5) gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	7918.79 (19)	7918.79 (19)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C32 H72 Cl Si8 U, C24 H48 Cl3 Mg2 O6 [+ solvent]	C32 H72 Cl Si8 U, C24 H48 Cl3 Mg2 O6	
Sum formula	C56 H120 Cl4 Mg2 O6 Si8 U [+ solvent]	C56 H120 Cl4 Mg2 O6 Si8 U	
Mr	1542.69	1542.68	
Dx, g cm ⁻³	1.294	1.294	
Z	4	4	
Mu (mm ⁻¹)	8.631	8.631	
F000	3200.0	3200.0	
F000'	3203.58		
h, k, lmax	16, 21, 40	16, 21, 40	
Nref	15035	21288	
Tmin, Tmax	0.302, 0.633	0.357, 0.661	
Tmin'	0.185		

Correction method= # Reported T Limits: Tmin=0.357 Tmax=0.661

AbsCorr = ANALYTICAL

Data completeness= 1.416

Theta(max)= 70.062

R(reflections)= 0.0828(15631)

wR2(reflections)=
0.2452(21288)

S = 1.014

Npar= 738

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

PLAT213_ALERT_2_C	Atom C5	has ADP max/min Ratio	3.3	oblate
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C33	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C41	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C34	Check
PLAT342_ALERT_3_C	Low	Bond Precision on C-C Bonds	0.01817	Ang.



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	13	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	6	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.19	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	11	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	3	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) U1 --Si1 .	6.4	s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	11%	Note
PLAT303_ALERT_2_G	Full Occupancy Atom H2 with # Connections	2.00	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H33B ..H36A .	2.09	Ang.
	x,y,z =	1_555	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	183	A**3
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	47	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed	!	Info
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.4	Low

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **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
11 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
7 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
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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.

