

## 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: I

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Bond precision:	= 0.0000 A	Wavelength=0.29060	
Cell:	a=6.4480 (8)	b=6.751 (2)	c=6.2630 (5)
	alpha=90	beta=102.063 (11)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	266.61 (9)	266.61 (9)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yabc	
	As0.17 Ce1.83 La0.84 Nd0.74		
Moiety formula	O16 P3.83 Pr0.20 Sm0.12	?	
	Th0.08, 0.1		
	As0.17 Ca0.19 Ce1.83 La0.84	Ce0.457 La0.21 Nd0.185	
Sum formula	Nd0.74 O16 P3.83 Pr0.20	Pr0.05 Ca0.047 Th0.02	
	Sm0.12 Th0.	Sm0.031 P0.958 As0	
Mr	939.71	234.90	
Dx, g cm-3	5.853	5.853	
Z	1	4	
Mu (mm-1)	6.370	6.451	
F000	419.8	420.0	
F000'	411.64		
h, k, lmax	14, 14, 13	13, 8, 13	
Nref	2954	773	
Tmin, Tmax		0.726, 1.000	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.726 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.262      Theta (max)= 18.600

R(reflections)= 0.0370( 741)

wR2(reflections)=

wR= 0.0476( 773)

S = 2.980

Npar= 36

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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.

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### Alert level A

EXPT005\_ALERT\_1\_A \_exptl\_crystal\_description is missing

Crystal habit description.

The following tests will not be performed.

CRYSR\_01

PLAT027\_ALERT\_3\_A \_diffrn\_reflths\_theta\_full value (too) Low ..... 9.61 Degree

PLAT029\_ALERT\_3\_A \_diffrn\_measured\_fraction\_theta\_full value Low . 0.470 Why?

PLAT699\_ALERT\_1\_A Missing \_exptl\_crystal\_description Value ..... Please Do !

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### Alert level C

GOODF01\_ALERT\_2\_C The least squares goodness of fit parameter lies  
outside the range 0.80 <> 2.00

Goodness of fit given = 2.980

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check

Calc: As0.04 Ca0.05 Ce0.46 La0.21 Nd0.18 O4 P0.96 Pr0.05 Sm0.03 Th

Rep.: Ce0.457 La0.21 Nd0.185 Pr0.05 Ca0.047 Th0.02 S

m0.031 P0.958 As0.042 O4

PLAT051\_ALERT\_1\_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 1.26 %

PLAT053\_ALERT\_1\_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054\_ALERT\_1\_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055\_ALERT\_1\_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077\_ALERT\_4\_C Unitcell Contains Non-integer Number of Atoms .. Please Check

PLAT127\_ALERT\_1\_C Implicit Hall Symbol Inconsistent with Explicit -P 2yabc Check

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### Alert level G

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 3 Info

PLAT005\_ALERT\_5\_G No Embedded Refinement Details Found in the CIF Please Do !

PLAT820\_ALERT\_5\_G Internal PLATON Read Problem with ALERT Number . \_820

PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.250 Check

PLAT068\_ALERT\_1\_G Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT092\_ALERT\_4\_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.29060 Ang.

PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check

PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of Th Constrained at 0.0199 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of Sm Constrained at 0.0312 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of Nd Constrained at 0.1848 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of Pr Constrained at 0.0503 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of Ce Constrained at 0.4566 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of La Constrained at 0.2104 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of As Constrained at 0.0416 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of P Constrained at 0.9584 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of Ca Constrained at 0.0467 Check

PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1)	33%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		100%	Note
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found			Please Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....			! Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .			Please Do !
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ		6	Units
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of		3.0	Sig(I)
PLAT984_ALERT_1_G	The Ce-f' = -2.0261	Deviates from the B&C-Value	-2.0173	Check
PLAT984_ALERT_1_G	The La-f' = -1.4695	Deviates from the B&C-Value	-1.4559	Check
PLAT984_ALERT_1_G	The Nd-f' = -3.1323	Deviates from the B&C-Value	-3.1595	Check
PLAT984_ALERT_1_G	The Pr-f' = -3.2550	Deviates from the B&C-Value	-3.2225	Check
PLAT984_ALERT_1_G	The Sm-f' = -2.0065	Deviates from the B&C-Value	-2.0091	Check
PLAT984_ALERT_1_G	The Th-f' = -0.9622	Deviates from the B&C-Value	-0.8911	Check
PLAT985_ALERT_1_G	The As-f" = 0.4019	Deviates from the B&C-Value	0.4005	Check
PLAT985_ALERT_1_G	The Ce-f" = 3.1615	Deviates from the B&C-Value	3.1748	Check
PLAT985_ALERT_1_G	The Nd-f" = 0.6212	Deviates from the B&C-Value	0.6180	Check
PLAT985_ALERT_1_G	The Pr-f" = 3.3462	Deviates from the B&C-Value	3.3560	Check
PLAT985_ALERT_1_G	The Sm-f" = 0.7152	Deviates from the B&C-Value	0.7111	Check
PLAT985_ALERT_1_G	The Th-f" = 3.4684	Deviates from the B&C-Value	3.4345	Check

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

26 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 1 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  
 12 ALERT type 4 Improvement, methodology, query or suggestion  
 7 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.

Datablock 1 - ellipsoid plot

