checkCIF/PLATON report

Structure factors have been supplied for datablock(s) wubin0112b1-5h

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: wubin0112b1-5h

Bond precision: O- C = 0.0120 A Wavelength=1.54184

Cell: a=5.0655(2) b=8.5990(3) c=7.3901(4)
alpha=90 beta=90 gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	321.90(2)	321.90(2)
Space group	P m c n	P m c n
Hall group	-P 2n 2a	-P 2n 2a
Moiety formula	C4 La1.80 Nd0.48 O16 Pb1.33 Pr0.32, 4(Sr0.02)	0.5(C4 La1.8 Nd0.48 O16 Pb1.32 Pr0.32 Sr0.08)
Sum formula	C4 La1.80 Nd0.48 O16 Pb1.33 Pr0.32 Sr0.08	C2 La0.90 Nd0.24 O8 Pb0.66 Pr0.16 Sr0.04
Mr	951.65	474.45
Dx,g cm-3	4.909	4.895
Z	1	2
Mu (mm-1)	103.486	103.159
F000	414.6	414.0
F000'	406.75	
h,k,lmax	6,10,9	6,10,9
Nref	382	379
Tmin,Tmax	0.427,0.539	0.148,1.000
Tmin'	0.310	

Correction method= # Reported T Limits: Tmin=0.148 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 77.109

R(reflections)= 0.0321(360)

wR2(reflections)= 0.0792(379)

S = 1.094 Npar= 34

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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ		Please Check
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..		2.75 Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..		Please Check
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)		O1 Check
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)		O2 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.037 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	2 Report
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.56Ang From O3	.	1.02 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.51Ang From O3	.	0.87 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.58Ang From O3	.	0.83 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.96Ang From O2	.	0.79 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.91Ang From O1	.	-1.04 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 1.07Ang From O2	.	-0.85 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 1.03Ang From O3	.	-0.65 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 1.02Ang From O3	.	-0.64 eA-3

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3 Info
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..		Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.500 Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		6.14 Why ?
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records		1 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		1 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of Pb1	Constrained at	0.3333 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Nd1	Constrained at	0.12 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Pr1	Constrained at	0.08 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of La1	Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Sr1	Constrained at	0.02 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)		24% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		100% Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		2 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		2 Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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 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
 10 ALERT type 4 Improvement, methodology, query or suggestion
  3 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.

PLATON version of 12/09/2022; check.def file version of 09/08/2022

Datablock wubin0112b1-5h - ellipsoid plot